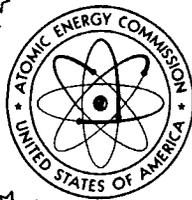


TID-4005 (Pt. 1, 8th Ed.)

**Summaries  
of the  
USAEC  
Basic Research  
Programs in  
Metallurgy,  
Solid State Physics  
and Ceramics**



(Fiscal Year 1964)

**United States  
Atomic Energy Commission  
Division of Technical Information**

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METALS, CERAMICS, AND MATERIALS  
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SUMMARIES OF THE USAEC BASIC RESEARCH  
PROGRAMS IN METALLURGY, SOLID STATE  
PHYSICS AND CERAMICS

January 1965  
[DTIE Issuance Date]



Division of Research, AEC  
Washington D. C.

## INTRODUCTION

Under the authority and direction of the Atomic Energy Act, the Atomic Energy Commission supports and fosters basic research related to its overall program. Virtually all such research is performed by contractor organizations. In addition to continuing programs in AEC-owned institutions, the Commission provides assistance to universities, other government laboratories, industrial laboratories, and others, who can contribute to the program of the Commission by research in their own laboratories.

While some basic research is, of necessity, performed in association with projects with applied objectives, the central effort of the Commission in the support of basic research in the physical sciences is the responsibility of the Division of Research. Under its auspices, research is being supported in the fields of high and low energy physics, chemistry, materials science, and controlled thermonuclear processes. This document summarizes the program on materials science supported by the Office of Metallurgy and Materials Programs of the Division of Research.

The function of the Metallurgy and Materials Programs is to support research conducted to advance the body of fundamental knowledge used to cope with the broad spectrum of materials problems facing nuclear technology. The approach taken is to investigate material structures, properties, and phenomena in the most rigorous possible fashion so that they may be explained, predicted, and related to the fundamental laws of nature. This content of the program embraces physical metallurgy and ceramics in their most basic context and solid state physics. Special importance is placed on advancing the understanding in detail of the effects of irradiation on materials and on the understanding of the structure and behavior of specific materials and materials classes of Commission interest.

In terms of the distribution of funds, about two-thirds of the Metallurgy and Materials Programs are conducted in the AEC laboratories. These are: Ames Laboratory, Iowa State University, Ames, Iowa; Argonne National Laboratory, Argonne, Illinois; Brookhaven National Laboratory, Upton, Long Island, New York; Lawrence Radiation Laboratory, University of California, Berkeley, California; Oak Ridge National Laboratory, Oak Ridge, Tennessee. Of the remaining one-third, most is spent in college and universities. At the end of the past fiscal year, June 30, 1964, the Office of the Metallurgy and Materials Programs was supporting 149 contracts in its contract research program. Of this total 140 were in 71 educational institutions and the balance in not-for-profit laboratories and industrial laboratories. The total expenditures were \$19,918,000 for Fiscal Year 1964.

Much of the research is conducted at the AEC laboratories since it requires experimental and support facilities not found elsewhere, such as high flux reactors and facilities for handling highly radioactive materials. Also, at the AEC laboratories concentrated efforts by relatively large numbers of mature scientists of many disciplines may be devoted to problem areas of long range Commission interest for extended periods of time.

The offsite contract research provides breadth and flexibility to the AEC program. By supporting such programs in universities, the AEC obtains the benefit of research conducted by those individuals who prefer an academic environment. For the most part, the offsite program is composed of small, short term projects. A major exception is the interdisciplinary laboratory at the University of Illinois where a single contract supports the research of a group of metallurgists, ceramists, chemists, and solid state physicists. In all the programs graduate student participation is an important factor.

The contracts supporting these offsite projects originate from unsolicited proposals based on the scientific interest of the principal investigator. Of the many such proposals submitted to the AEC, those chosen for funding are selected on the basis of their scientific merit and their pertinence to the AEC program. The resulting contracts usually cover a one-year period but may be renewed if the research continues to be productive and of AEC interest, and if sufficient funds are available.

This report contains summaries of the research programs active during Fiscal Year 1964. Part I presents the research conducted in the AEC laboratories and Part II, the research conducted elsewhere. For the most part, these summaries were written by the investigators themselves. However, some editing has been done for consistency of format. The summaries have been indexed in terms of senior technical people involved and in terms of scientific content.

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PART I  
RESEARCH IN AEC LABORATORIES



The deoxidation of niobium and vanadium by treatment with the alkaline earth metals at 1000-1200°C gives equilibrium concentrations of oxygen of 40 ppm or less. Experiments designed to decrease carbon and other interstitial impurities in vanadium to very low concentrations by a special hydrogen treatment, such as has been used successfully on iron, is underway. Preparation of vanadium and niobium by reduction of their oxides with high purity aluminum followed by iodide refining or electron beam melting shows considerable promise as a simplified process for obtaining these metals in pure form.

## 2. Imperfection Structure and Relationship to Properties

F. X. Kayser and M. J. Marcinkowski

A study of dislocation structures in crystals using transmission electron microscopic techniques has been initiated. The interaction between dislocations resulting from antiferromagnetic ordering in the compound, FeRh, and accompanying work hardening in the ferromagnetic super-lattice alloy, FeCo is being investigated. The relationship between imperfection structure and superconductivity in thin films is also of interest. Measurement of stacking fault energies of several rare-earth metals and a study of diffusion-induced effects in thin foils are underway.

Investigation of the "k state" in Cr-Ni alloys is in progress with efforts to interpret the observed phenomenon by correlation with the dislocation structure of the alloys.

## 3. Mechanical Properties of Metals & Alloys

O. N. Carlson, F. X. Kayser, M. J. Marcinkowski, D. T. Peterson and T. E. Scott

A better understanding of the deformation process in metals and the effect of impurities on strength and ductility constitute the major objectives of this research program. The role of impurities in the brittle-ductile transition and also in the strain aging phenomenon in body-centered cubic metals is of specific interest. The effect of nitrogen on the brittle-ductile transition of vanadium and chromium has been studied rather extensively. Activation energies associated with strain aging in these metals were found to be in rather good agreement with the reported values for diffusion of nitrogen in these metals. The deformation mechanisms of tantalum and niobium at sub-atmospheric temperatures were determined and attempts made to explain the difference in the brittle-ductile behavior of these metals on the basis of these observations. The strain rate-temperature-ductility relationships for vanadium and vanadium-hydrogen alloys are being determined.

Fcc thorium exhibits a pronounced yield point at room temperature at stresses as low as 12,000 psi. The temperature and strain rate dependence of the flow stress of thorium is quite unusual and interesting for a fcc metal. The creep rate is being studied as a function of temperature and stress.

An investigation of the peculiarities in the plastic behavior of off-stoichiometric, long-range ordered Fe<sub>3</sub>Al alloys is in progress. Aluminum-rich alloys show yield points at room temperature while those on the iron-rich side of the compound do not. Metallographic and surface replication procedures have been developed and single crystals of the composition of interest grown.

#### 4. Thermodynamic Properties of Alloys

P. Chiotti, F. X. Kayser, K. A. Gschneidner, D. T. Peterson, J. F. Smith

The thermodynamic properties of intermetallic compounds, metallic solutions and metal-salt systems are being investigated by calorimetric, vapor pressure and electromotive force measurements. Attempts are being made to relate thermodynamic properties to the atomic structure and other properties of the alloy.

A transformation has been established in  $\text{YZn}_2$  and the enthalpy change and other characteristics of the transformation measured.

The heats of fusion of zinc and bismuth and the heats of formation for  $\text{CaMg}_2$  were determined and the heat contents of tantalum and  $\text{Na}_x\text{WO}_3$  ( $x \approx 0.65$ ) were determined from 0 to 1100°C and 0 to 700°C respectively.

The activities and activity coefficients of  $\text{ZnCl}_2$  in  $\text{KCl-LiCl}$  were measured for various concentrations over the temperature range 450-650° as were the thermodynamic properties of liquid  $\text{MgZn}$  alloys.

The vapor pressures of calcium, barium and strontium were determined by the Knudsen effusion method as a function of the metal concentration in solutions of their respective molten chlorides. The observed concentration dependence of the vapor pressure indicates that two solute particles are formed for each atom of metal in solution.

Calcium-ytterbium alloys are being used to study whether short range ordering or clustering exists in their solid solutions by diffuse x-ray scattering techniques. A study of the Ca-Yb phase system has been initiated with particular emphasis on the limits of terminal solid solubility.

#### 5. Kinetics of Metallurgical Reactions

D. T. Peterson and J. D. Verhoeven

Diffusion of solutes in solid and liquid metal systems and the migration of solutes under influence of electric field and thermal gradients are being measured.

A technique has been developed for producing a liquid zone in 1/2-inch diameter rods of iron and yttrium with a direct current of up to 700 amperes per  $\text{cm}^2$  for use in studying the transport of solute atoms under the combined potential and thermal gradients. Normal freezing experiments have been carried out with a current of 250 amperes per  $\text{cm}^2$  passing through the liquid-solid interface of a bismuth-tin eutectic alloy. A study of resistivity and convection effects in liquid metals is also underway.

Rates of diffusion of hydrogen in barium and in the divalent rare-earth elements, Eu and Yb, are being measured and the kinetics of the oxidation of thorium is being determined.

## 6. Phase Formation, Structure and Stability of Alloys

J. F. Smith

This area of research includes a study of the stability and crystallography of intermetallic compounds and other intermediate phases in alloy systems using elastic constant and magnetic susceptibility measurements and x-ray diffraction techniques.

The crystal structures of  $\text{YNi}$ ,  $\alpha\text{-YAl}_3$ ,  $\text{YMg}_2$ ,  $\text{Y}_4\text{Mg}_{25}$  and  $\text{NbSn}_2$  have been determined and space groups determined for  $\text{YNi}_3$ ,  $\beta\text{-YAl}_3$ ,  $\text{Nb}_6\text{Sn}_5$  and  $\text{Th}_6\text{Mg}_{23}$ . The structures of  $\text{CaZn}_5$  and  $\text{CaZn}_{13}$  have also been confirmed. The elastic stiffness constants of the fcc phase in the thallium - indium system were measured on single crystal alloys as a function of temperature and composition. Measurement of the elastic constants of single crystalline rhenium as a function of temperature is in progress and the elastic constants for  $\text{UCd}_{11}$  have been determined.

Measurement of the anisotropic thermal expansion of indium over the temperature range 80-300°K was made for different grades of indium and for its dilute alloys. Magnetic susceptibilities were determined for a group of intermetallic phases all of which have the fluorite structure. The phases investigated were of the series  $\text{AuAl}_2$ ,  $\text{AuIn}_2$  and  $\text{AuGa}_2$  and the analogous series  $\text{MgSi}_2$ ,  $\text{MgGe}_2$ ,  $\text{MgSn}_2$  and  $\text{MgPb}_2$ .

## 7. Properties and Alloy Behavior of the Rare-Earth Metals

K. A. Gschneidner and F. H. Spedding

The purpose of this program is to investigate the physical properties, electronic structures and alloy behavior of the rare-earth metals. The major objective of this work is to obtain a basic understanding of the metallic state and to extend our knowledge of alloy theory from a study of this closely related series of elements.

A study of the electronic transition in cerium, the band structure of its various allotropes and the effect of alloying upon these transformations is underway. Binary alloys of neodymium and yttrium were found to have the unique "samarium" structure whereas neodymium-scandium alloys do not exhibit this behavior, presumably due to atomic size factors. Studies of the scandium-gadolinium and scandium-yttrium systems indicate that the difference in the electronic structures of yttrium and gadolinium does not result in any observable difference in the phases present at elevated temperatures. The solubility limits of magnesium in the rare earths and of these metals in gold are being determined as part of a study of the nature of solid solution alloying.

The magnetic properties of  $\text{YMn}_4$  when scandium is substituted for yttrium in various proportions, is of interest in understanding the unusual ferromagnetic behavior of this compound. Unusual magnetic properties were also observed in several non-stoichiometric rare-earth oxides having the formula,  $\text{M}_{33}\text{O}_{48}$ . Single crystals of these oxides have been prepared for use in these studies.

Work is continuing on measuring the vapor pressures and high temperature heat contents of the rare-earth metals and is being extended to their intermetallic compounds and other binary systems.

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Encyclopedia of Chemical Technology, Vol. 3  
Interscience Publishers, New York, N.Y. (1963)

Theodore Martin Brown and Robert E. McCarley  
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U. S. Atomic Energy Comm. Rept. IS0741, Nov. 1963.

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The Preparation of  $TaBr_4$ ,  $TaI_4$  and Pyridine Adducts of the Tantalum (IV) Halides  
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X-Ray and Ultrasonic Techniques  
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Elastic Constants of Thallium Single Crystals in the Temperature Range 4.2 - 300°K  
J. Appl. Phys. 34 (1963) p. 768.

B. J. Beaudry and A. H. Daane  
The Sc-Y and Sc-Zr Systems  
Trans. Met. Soc. AIME 227, (1963) p. 865.

W. J. Wunderlin, B. J. Beaudry and A. H. Daane  
The Solid Solubility of Holmium in Copper, Silver and Gold  
Trans. Met. Soc. AIME 227, (1963) p. 1302.

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Electron Requirements of Bonds in Metal Borides  
J. Chem. Phys., 38, (1963) p. 425.

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Present Contract Term: July 1, 1963 to June 30, 1968

Cost to AEC: \$1,290,000 (FY 1964)

Contract Title: BASIC RESEARCH IN THE SOLID STATE DIVISION

Investigators: F. H. Spedding, D. J. Zaffarano, and Staff

Scope of Work:

A. Electronic Properties of Metals

A. V. Gold, J. M. Keller, A. R. Mackintosh, R. C. Young, and D. J. Zaffarano

The details of the Fermi surfaces of both transition and nontransition metals are being investigated using a number of different techniques. Pulsed magnetic fields of up to 200 kilogauss have been used to study the de Haas-van Alphen effect in lead as well as in tungsten, molybdenum, and single crystal "whiskers" of the ferromagnetic metals iron and cobalt. The experimental band structure for lead is well understood from the standpoint of the nearly-free electron model. The theoretical interpretation of the results for the transition metals is much more complicated, since the simple model does not appear to apply in this case. Other related investigations include the magneto-acoustic effect in white tin, angular correlation of the annihilation gamma rays for various metals (such as chromium), and cyclotron resonance at 100 kmc/s in tin and thallium.

The measurements on iron and cobalt offer a means for studying the internal magnetic fields in these metals, and the internal fields are being investigated also by means of magneto-resistance and Hall effect measurements on the "whiskers". Various theoretical approaches to this problem are being considered.

B. Electronic Structure of Crystalline Solids

R. G. Barnes

Nuclear magnetic resonance (NMR), electron spin resonance (ESR) and recoilless-resonance absorption of gamma radiation (Mössbauer effect) are being used to investigate nuclear hyperfine interactions in solids, with the emphasis being on pure metals, alloys and intermetallic compounds. Experimental NMR studies have been completed on the In(115), La(139), Sc(45) and Be(9) nuclei in the pure metals, and these are being interpreted theoretically. Results which have been obtained for vanadium metal strongly suggest that the

influence of gaseous impurities is responsible for the failure to detect NMR in a number of other transition metals. The effects of magnetic ordering have been studied in the vanadium-chromium system, and similar work is in progress in the rare earth-aluminum compounds of the form  $RA_2$ . These investigations will be extended to similar tin compounds using the Mössbauer effect. A combination of high pressure and NMR techniques is being used to obtain the activation volumes for self-diffusion in aluminum, and in lithium-magnesium alloys. ESR work to date has been concerned with an investigation of the  $V^{4+}$  and  $Mn^{4+}$  ions in rutile ( $TiO_2$ ), and with the effects of rare earth ions in  $CdF_2$ . Some non-stoichiometric compounds of the  $Li_xWO_3$  type have been studied also.

### C. Cryophysics: Superconductivity

#### 1. Superconductivity

D. K. Finnemore, F. H. Spedding, and C. A. Swenson

This program involves primarily an investigation of the superconducting properties of high purity transition metals, and the effects on the superconducting properties of these metals of alloying with known amounts of both magnetic and nonmagnetic metals. Magnetization curves which show type II behavior have been obtained for high purity niobium at temperatures up to  $9^{\circ}K$ . Various other high purity transition metals (thorium, vanadium) are being studied in an effort to ascertain their thermodynamic and superconducting properties. The changes in the superconducting behavior of high purity lanthanum metal upon alloying with small amounts of gadolinium have been studied using magnetization curves, resistivity, and heat capacity. Considerable evidence for the existence of gapless superconductivity has been found in a rapid decrease to zero of the magnitude of the specific heat jump at  $T_c$  as the gadolinium concentration is increased from zero to approximately 0.5 percent.

#### 2. Specific Heat Measurements Below $1^{\circ}K$

F. H. Spedding, C. A. Swenson

A magnetic refrigerator has been constructed for heat capacity measurements at temperatures from  $0.15^{\circ}K$  to  $20^{\circ}K$ . Initially, data are being obtained for both isotopes of solid helium at pressures up to 2 kbars, and for high purity rare earth metals, where the hyperfine interaction terms will be of major interest.

### D. Thermal and Thermodynamic Properties of Solids

#### 1. Equation of State Studies

C. A. Swenson

The piston-displacement method is being used to obtain pressure-volume-temperature measurements for simple solids (such as potassium metal) which are of direct theoretical interest, and for more complex substances (such as terbium metal,  $MnSn_2$ ,  $NH_4F$ ) for which such data do not exist. The major

objectives involve, first, an understanding of the pressure-volume relationship at absolute zero, and, second, the influence on the temperature-dependent portion of the equation of state of both lattice and magnetic properties. Low temperature thermal expansion measurements are being made from 1.2°K to 30°K using an apparatus which can detect changes in the length of the order of 0.1 Angstrom in a 10 cm long sample. Data which have been obtained for copper and aluminum confirm those published by other laboratories, while both sapphire and rubidium iodide have shown anomalous behavior.

## 2. High Temperature Measurements

G. C. Danielson

Pulsed techniques are being used to measure the thermal diffusivity and specific heat of various solids from 300°K to 1400°K, and a new radial geometry method for the thermal diffusivity measurements has been developed. Various pure metals and semiconductors are being studied.

## 3. Theory

J. M. Keller, R. H. Good

A general interest in the lattice properties of solids is reflected in rather diverse types of calculations. Anharmonic effects in the specific heats of solids are being studied in both the high temperature and low temperature limits, the latter being specifically concerned with the heat capacity of solid helium. The proper formulation of the local energy flux operator and a statistical description of a system in a temperature gradient are being studied for a semi-infinite chain, in the hopes of understanding more completely the fundamental problem of heat conduction in a solid.

A model which uses a free-electron representation for the conduction electrons has been used to study the energy of the metallic state for a number of elements. The results for the alkali and alkaline earth metals are most successful.

## 4. Mass Spectrometric Techniques

D. E. Hudson

These techniques have been used to study surface ionization, ionization cross-sections for electron bombardment, and relative vapor pressures (cohesive energies). Recent work has been confined to various rare earth metals.

### E. Semiconductors and Compounds with Variable Stoichiometry

#### 1. Semiconductors

G. C. Danielson, D. E. Hudson, J. M. Keller, D. W. Lynch, and R. C. Young

The major research in this area is concerned with the series of intermetallic compounds of the form  $Mg_2X$ , where X represents Ge, Si, Sn and Pb.

The emphasis has been on single crystals of  $Mg_2Si$  and  $Mg_2Ge$ , where various measurements (electrical resistivity, Seebeck coefficient, Hall effect, magnetoresistance, elastic constant, specific heat, optical reflectivity, high pressure resistivity) have been made in order to understand their basic properties. In particular, piezo-resistance measurements on n-type  $Mg_2Si$  indicate that it is a multivalley semiconductor with a structure similar to silicon. The band structure of  $Mg_2Si$  is being calculated. Microwave Hall mobility measurements have been made on germanium at 10 kmc/s, and higher frequency measurements have been initiated to extend these measurements and cyclotron resonance measurements to 100 kmc/s.

The true bulk resistivity of diamond has been determined, and its temperature dependence suggests that both deep and shallow donors are present.

## 2. Tungsten Bronzes

G. C. Danielson, R. Fuchs, D. W. Lynch, and A. R. Mackintosh

The sodium and lithium tungsten bronzes (of the form  $Na_xWO_3$ , where x is less than unity and is variable over certain ranges with constant crystal structure) form a class of metals where the conduction electron density can be varied, and where a transition from metallic to semiconducting behavior is found. Many of their observed properties can be understood in terms of a diffusion model, and an approximate band structure for these has been proposed. Recent measurements have included optical reflectivity and specific heats down to 10°K.

## F. Magnetic Materials; Rare Earth Metals and Rare Earth Compounds

### 1. Rare Earth Single Crystals

S. Legvold, A. R. Mackintosh, and F. H. Spedding

The availability of high purity single crystals of the rare earth metals has allowed detailed investigations to be made of their interesting anisotropic magnetic properties. The data furnished by neutron diffraction experiments performed elsewhere complements the single crystal magnetization, electrical resistivity, thermoelectric power and magnetostriction measurements which are currently being made. The very large magnetostriction effects which have been found for dysprosium and holmium must be related, for instance, to the large magnetic anisotropies in these substances. The complex magnetic structure of these elements also is apparent in magnetoresistance measurements.

### 2. Rare Earth Ethyl Sulfates

F. H. Spedding, R. H. Good

The absorption spectra of the rare earth ions in single crystals of rare earth ethyl sulfates have been investigated with high resolution as functions of temperature, magnetic field and crystal orientation. These data give details about the crystal field environment of the rare earth ion which

have not been measurable before. The results can be understood in terms of a theory which has been developed for the Zeeman effects of rare earth ions in crystal fields with  $C_{3h}$  symmetry.

#### G. Ionic Crystals and Color Centers

D. W. Lynch, R. Fuchs, and K. L. Kliever

##### 1. Experimental

D. W. Lynch

Color centers in the cesium halides are being studied by both absorption and luminescence techniques. A system has been constructed to study the effects of 4 kbars pressure at liquid nitrogen temperatures on luminescence from color centers, and preliminary data have been obtained for KCl. The analysis of ionic conductivity data to obtain defect mobilities in AgCl and AgBr has been simplified by means of a Born-Mayer model calculation of the binding energy of a silver vacancy to a divalent metal impurity.

##### 2. Theory

R. Fuchs, K. L. Kliever

A direct calculation of the energy levels of the A center in KCl is being carried out using a direct calculation of the pseudopotentials. The pressure and temperature dependences of the static dielectric constants of alkali halides are being calculated in such a manner that the effect of each parameter used to characterize a particular crystal (e.g., ionic masses, polarizabilities) will be made apparent.

The effect on various crystal properties of markedly nonhomogeneous defect distribution near surfaces and around dislocations in alkali halide and silver halide crystals (e.g., ionic conductivity) is being investigated.

#### H. Neutron Scattering Experiments

K. L. Kliever, A. R. Mackintosh

The Ames Laboratory Research Reactor will be used initially for the determination of spin-wave and phonon spectra in various solids when it comes into operation early in 1965. Plans also are being made for the use of elastic neutron scattering techniques for the determination of magnetic spin distributions in magnetically ordered solids.

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Contractor: Argonne National Laboratory, Argonne, Illinois

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Contract Title: PHYSICAL RESEARCH IN THE METALLURGY DIVISION

Investigators: H. H. Chiswik, Associate Director, Metallurgy Division

Scope of Work:

The scope and objectives of this program encompass the following:

(a) Studies to determine and correlate the physical and mechanical properties of the materials that are basic to reactor technology in terms of their atomic and electronic structure; in support of this there are programs dealing with the physical metallurgy of plutonium, uranium, zirconium, and their alloys.

(b) Studies designed to extend our knowledge and understanding of the mechanisms and processes which are usually encountered in metallurgical and ceramic technology and which have a special and unique significance in nuclear technology; included are such processes as corrosion, diffusion, structures of thin films, effects of surface structure on chemical reactivity, mechanisms of phase transformations, and interactions of dislocations and their effects on mechanical properties.

(c) Studies on alloying properties of transition metals, both solid solutions and intermediate phases, with emphasis on the electronic properties and their role in determining the stability of phases, utilizing such measurements and techniques as nuclear magnetic resonance, low temperature specific heat, and magnetic susceptibility.

(d) Diffraction studies by combined neutron and X-ray techniques on the determination of nuclear, atomic, and structural properties of materials, with increasing emphasis on neutron diffraction.

(e) Studies on irradiation effects in metals and alloy systems designed to shed light on the nature of irradiation induced damage. The design and construction

of low temperature facilities have been completed. These are located in the CP-5 reactor and allow bombardments to temperatures as low as 3.5°K in a thermal neutron environment of  $2.5 \times 10^{13}$  neutrons per  $\text{cm}^2$  per second and less than  $10^{10}$  neutrons per  $\text{cm}^2$  per second of epithermal or higher, or in a neutron environment of  $3 \times 10^{11}$  fission neutrons with less than  $10^8$  thermal neutrons. The scope of the research involves a variety of in situ measurements including stored energy, electrical resistivity, length change measurements in nonfissile metals, such as the noble metals, especially with regard to dose dependence effects in the high dose regions. Currently experiments to measure the radiation-induced electrical resistivity as a function of neutron dose are under way. A joint research effort with Dr. C. S. Barrett of the University of Chicago to measure the recovery of radiation-induced changes in lattice parameter is also under way.

#### A. Physical Metallurgy of Basic Reactor Materials (L. T. Lloyd)

##### 1. Plutonium Physical Metallurgy (L. T. Lloyd, A. F. Berndt, M. B. Brodsky, R. Liptai)

High-Purity Metal: Preparation of high-purity plutonium by electrolysis in a fused salt electrolyte is being continued to provide material for our research studies.

Deformation and Recrystallization: In connection with studies on the recrystallization and grain growth in alpha plutonium, a procedure has been developed whereby this previously considered brittle and unworkable phase can be flat rolled as much as 99% reduction in thickness at room temperature without intermediate thermal treatments. The rolling introduces preferred orientation into the material, but the amount of stored energy is small. In fact, the hardness of the material after rolling more than 80% reduction in thickness is less than before rolling. Annealing the rolled material within the temperature range of the alpha phase (up to about 120°C) does not bring about recrystallization, but annealing samples rolled approximately 85% reduction in thickness at temperatures above the equilibrium  $\alpha \rightarrow \beta$  transformation temperature for short periods of time that are insufficient to permit the transformation to occur does result in recrystallization without appreciable grain growth.

Self-Irradiation Damage: To determine the effect of self-irradiation damage due to radioactive decay on the flow stress in alpha plutonium, hardness measurements at room temperature have been made on samples held for various periods of time at liquid nitrogen (77°K) and liquid helium (4.2°K) temperatures. In most cases, the hardness decreased with holding time.

Single Crystal Preparation: Several approaches to the problem of preparing single crystals of monoclinic alpha plutonium are under investigation. These include: 1) Electrolytic reduction of plutonium halides, 2) growth from solutions in liquid alkali metals, 3) reduction of plutonium halides by lithium in non-aqueous solutions; and 4) studies of the grain structures in samples cooled from a high temperature phase at both atmospheric and slightly elevated pressures.

Equipment is being procured to extend the range of hydrostatic pressures to 100 kilobars at temperatures up to approximately 1000°K. An extrapolation of reported data for the P-T diagram of plutonium indicates that liquid plutonium might solidify directly to the alpha phase at these pressures. The equipment will also be used for studies of other pressure effects in plutonium and other actinide metals.

Crystal Structure: Proof of the indexing of powder patterns and determination of the unit cell of alpha plutonium was provided by an X-ray study of a small single crystal of a plutonium-neptunium alloy which had the crystal structure of the alpha plutonium phase.

Alpha  $\rightleftharpoons$  Beta Transformation: The kinetics of the  $\beta \rightarrow \alpha$  transformation in high-purity plutonium have been studied by ultrasonic measurements of samples isothermally treated at various temperatures from 191° to 361°K. The TTT diagram shows a double "C" character. The upper "C" (313° to 361°K) is accompanied by a partial athermal character in that the transformation does not go to completion, but rather, the amount of transformed material approaches a certain value and further holding time has no effect. Upon subsequent cooling to room temperature, the transformation goes to completion. The lower "C" shows a minimum time for beginning of transformation of approximately 0.5 sec at approximately 270°K.

Transport Properties: A study is in progress on the electron transport properties of plutonium and other actinide metals and their alloys. Thus far, measurements have been made of the Hall coefficient of plutonium between 78° and 438°K, and of the electrical resistivity of cold-rolled alpha plutonium between 4.2° and 393°K. The Hall coefficient of alpha plutonium was found to change from a positive value above 190°K to a negative value below that temperature. The Hall coefficients for beta plutonium, however, are positive throughout the temperature ranges studied (78° - 160°K and 353° - 438°K). The results have been treated by a two-band model which yields consistent results if the conduction band is assumed to be 7s, but the results are not consistent with an assumed 6d conduction band. Differences in calculated band populations between the alpha and beta phases imply slight differences in the band structures of the two phases.

Measurements of the low temperature resistivity of rolled plutonium have shown that the resistivity anomalies are affected by the deformation, but they are not totally eliminated by it. The rolled metal gives better resistivity ratios than previously reported, but these are still quite low. The results on the cold-rolled metal are in agreement with proposed antiferromagnetic ordering below 60°K.

## 2. Diffusion Studies (S. J. Rothman and N. Peterson)

Studies of diffusion of  $U^{235}$  and of  $U^{233}$  in perfect and imperfect single crystals of alpha-uranium are in progress to determine the temperature dependence of D, and the effect of dislocations on the diffusion rate.

The measurements of the diffusion of Zn in NaCl, made by one of us at Harwell last year (Rothman), have been analyzed. For the diffusion of Zn in pure NaCl,  $D_0$  was  $2 \times 10^{-2}$  cm<sup>2</sup>/sec and the activation energy was 23.8 kcal/mol. The energy of association between a Zn<sup>++</sup> ion and a nearest-neighbor cation vacancy was 15.6 kcal/mol, and the heat of solution of ZnCl<sub>2</sub> in NaCl was 27 kcal/mol. Zn diffuses in NaCl by the vacancy mechanism.

Diffusion of Pd<sup>103</sup> has been measured in single crystals of copper and silver. The temperature dependence of the diffusion coefficient may be represented by:

$$D_{\text{Pd} \rightarrow \text{Ag}} = 9.57_{-1.37}^{+1.63} \exp[-(56,752 \pm 300)/RT] \text{ cm}^2/\text{sec},$$

and

$$D_{\text{Pd} \rightarrow \text{Cu}} = 1.71_{-0.21}^{+0.23} \exp[-(54,370 \pm 300)/RT] \text{ cm}^2/\text{sec},$$

where R is the gas constant and T is the temperature in °K. The results, when compared with the activation energies for self-diffusion in copper and silver, are in poor agreement with the LeClaire theory. One may conclude that the electrostatic potential due to an electronegative impurity dissolved in a noble metal cannot be described by the Thomas-Fermi potential. From the Lidiard theory, this data, and data of Nachtrieb et al., the correlation factor for palladium diffusion in silver has been shown to be 0.96 and 0.98 at 1203° and 1023°K, respectively. It may further be shown that palladium atoms repel vacancies in both the first and second coordination shells.

Simultaneous diffusion of Pd<sup>103</sup> and Pd<sup>112</sup> has been measured in palladium single crystals. The preliminary results for Pd<sup>103</sup> diffusing in Pd can be represented by:

$$D = 0.1 \exp(-62,000/RT) \text{ cm}^2/\text{sec}.$$

The isotope effect in palladium self-diffusion has been measured to within approximately 5%. The square root of mass dependence of the diffusion coefficients is found to hold within this experimental accuracy. The isotope effect on palladium diffusion in copper and silver is now being investigated. The correlation factor obtained with this work will then be compared to the values obtained with the Lidiard theory in our earlier experiments.

### 3. Elastic Constants and Their Relation to HCP to BCC Transformations (E. Fisher)

For crystals of hexagonal symmetry there are two fundamental elastic shear moduli,  $c_{44}$  and  $c_{66}$ . The  $c_{44}$  modulus associates the stress and strain for shear in the basal planes, whereas the latter is the modulus for prism shear or shear of any (h·k·0)[h·k·0] system. Measurements of the elastic moduli in Ti and Zr

have shown that the  $c_{66}$  moduli in these two h.c.p. metals have almost the same values between 4°K and the respective temperatures of the h.c.p.  $\rightarrow$  b.c.c. diffusionless transformations, 1135° and 1155°K. In addition, the  $c_{66}$  moduli have a much greater temperature dependence than  $c_{44}$  of either metal. In Hf and Y,  $c_{66}$  also has the larger temperature dependence.

In correlating the relative temperature dependence of the two shear moduli with the  $c/a$  ratios of h.c.p. metals at 298°K, it was found that for Cd, Zn, Co, and Mg, with  $c/a$  values greater than 1.60, the  $c_{44}$  modulus has either the same or a greater temperature dependence than  $c_{66}$ . For  $c/a$  values less than 1.60, however, which includes Tl, Zr, Ti, Hf, Y, Be, a number of rare earth metals and the platinum group members, Ru and Os,  $c_{66}$  has the greater temperature dependence, except Ru (data are not available for the rare earths, nor for Os). A further correlation shows that  $c/a$  of about 1.60 is also the dividing point, distinguishing between those h.c.p. metals which transform to b.c.c. before melting and those which do not. Two exceptions were noted: Ru and its associate Os.

This correlation suggests that the occurrence of the h.c.p. to b.c.c. transformation is associated with the temperature dependence of the thermal vibrational amplitudes, corresponding to the transverse modes, with displacements in the h.c.p. basal planes. The elastic constant data together with the electrical resistivity and specific heat data (literature data) suggest that above 420°K these thermal displacements are impeded by anharmonicity in the lattice vibrations which contribute to a high vibrational free energy that is greater than that obtained from a quasi-harmonic model.

The temperature dependence of the nine elastic moduli in orthorhombic alpha uranium are being measured up to temperatures close to the  $\alpha \rightarrow \beta$  phase transformation. The data obtained for the shear moduli are quite similar to those observed in Ti and Zr, in the range of 100° to 400°K, but do not show evidence of anharmonicity in the 400° to 900°K range. In fact, the data at high temperatures suggest that the negative thermal expansion coefficient of the  $b_0$  lattice constant in uranium is associated with an increasing temperature dependence of the amplitudes for the transverse modes of thermal vibration.

#### 4. Precipitation Strengthening of Alpha-Zirconium Crystals by Hydrogen (D. Westlake)

Transmission electron microscopy has been used to study the location of hydrogen in quenched zirconium-hydrogen alloys. Contrary to published results of other workers, hydrogen in interstitial solid solution at 573°K was not retained in supersaturated solution by quenching in water. Freshly quenched alloys contained finely dispersed needles of zirconium hydride, which increased in size during aging at room temperature. Some precipitates were formed at dislocations, but nucleation sites appeared to be randomly distributed in the matrix.

The critical resolved shear stress for prism slip of crystals of zone refined zirconium was increased as much as 500 per cent by 0.54 a/o hydrogen in the form of finely dispersed hydride needles. The combined strength increment due to hydrogen and the impurity, oxygen, is expressed by

$$\Delta\tau = (\tau_H^2 + \tau_O^2)^{1/2},$$

where  $\tau_H$  and  $\tau_O$  are the increments of strength due to hydrogen and oxygen, respectively. This is in agreement with a recently published theory for strengthening due to two causes. The increment  $\tau_O$  was shown to be equal to  $(A-BT^2/3)^{3/2}$ , and  $\tau_H$  was equal to  $KG$ , where  $A$ ,  $B$  and  $K$  are constants,  $T$  is temperature in  $^{\circ}K$ , and  $G$  is the shear modulus. One deduces from this that glide dislocations overcome oxygen barriers by a thermally activated process, but the mechanism of overcoming hydride barriers is not thermally activated.

## B. Alloy Studies (M. V. Nevitt)

### 1. Occurrence of Transition Element Intermediate Phases (A. E. Dwight)

Currently a major part of this investigation is concerned with the factors which control the occurrence of various crystal structures in equiatomic alloys. In these alloys, the A partner comes from a group in the periodic table to the left of the Mn group, and the B partner comes from a group to the right of Mn.

The B2, or CsCl-type structure, occurs in more than 170 binary systems. Atomic size, as measured by the Goldschmidt radii of the partners, is not a major controlling factor. The operation of an electronegativity factor may be important, as is shown by the transition from a disordered A2 solid solution in TiRe to a B2 structure, by the substitution of successively smaller amounts of Os, Ir or Pt for a part of the Re. A study of the interatomic contraction in B2 compounds shows that contraction between the A and B partners is dependent upon radius ratio and group number of the A and B partners. When the B element is from the second long period, contraction is noticeably less than when the B element is from the third long period.

The B27, or FeB-type, has been found in alloys in which the A element is a lanthanide or Th, and the B element is Ni, Pd, Pt, Cu or Si. The Bf, or CrB-type, structure has been found in alloys in which the A element is a member of the Ca, Sc, Ti or actinide group, and the B element is Ru, Co, Rh, Ir, Ni, Pt, Al, Ga, Si, Ge or Sn. Both structures are orthorhombic and both are accompanied by large radius ratios. The factor which controls the selection between a B27 and Bf structure is not yet known.

The B19 structure is found in equiatomic compounds which have a moderate radius ratio and whose B element is Pd or Pt; newly discovered examples are TiPd and TiPt.

The  $L1_0$ , or CuAu-type, is most prevalent in systems having a low radius ratio and small differences in electronegativity. A recently found example in a ternary system is  $V_2IrPt$ . The transition of an  $L1_0$  structure to a distorted  $B2$  has been studied.

The  $B11$  structure, which is ordered tetragonal, has been found more often in ternary than in binary systems. A typical ternary  $B11$  compound is  $Ti_3Hf_7Ir_{10}$ .

A graphical scheme has been devised which enables one to gather compounds having a common crystal structure into regions of composition. The occurrence and composition of a given crystal structure family can thereby be related to the position of the partner elements in the periodic table. The graphical scheme of presentation has particular usefulness in predicting occurrence of compounds in certain ternary systems.

## 2. Phase Relationships in Systems of Actinide Elements with Carbon (M. V. Nevitt)

The principal effort here has been an X-ray diffraction study of NaCl-type monocarbides of thorium, uranium, neptunium and plutonium and solid solutions formed between them. The X-ray work has been supplemented by optical metallography. The effort has been confined to four specific areas:

a. The composition limits and the concentration dependence of the lattice parameter have been determined for the binary phases  $\overline{ThC^*}$ ,  $\overline{PuC}$ , and  $\overline{NpC}$ . As these phases form over a range of composition (deficient in carbon in relation to ideal stoichiometry) it has been possible to derive empirically expressions relating the lattice parameters to the ratio of atom fraction of carbon to the atom fraction of the metal.

b. The lattice parameters of the  $\overline{(Th,U)C}$  and  $\overline{(Th,Pu)C}$  phases have been determined after samples were reannealed at high temperatures. There is complete miscibility between the carbides involved and the relationships between lattice parameters and composition does not differ appreciably from linearity.

c. The approximate composition range of  $\overline{(Th,Np)C}$  has been explored and certain other pertinent phase relations have been tentatively established. The lattice parameter of the  $\overline{(Th,Np)C}$  phase has been measured. The results thus far obtained suggest, but do not prove conclusively, that  $\overline{NpC}$  is completely soluble in  $\overline{ThC}$ .

d. A tentative interpretation of the lattice parameters of the binary monocarbides has been made in terms of the relationship between valence and atomic-radius which is characteristic of the actinide series. Although the sizes of the atoms in the structures of pure uranium, neptunium and plutonium indicate that the number of electrons in 7s and 6d states (valence electrons) is respectively 6, 6, and 5, their effective size in the carbides suggests a smaller number. We infer that the

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\* The symbols  $\overline{ThC}$ ,  $\overline{NpC}$ ,  $\overline{PuC}$ ,  $\overline{(Th,Np)C}$ , etc., are used to denote the phases without implying stoichiometry.

effective atomic size corresponds to between 4 and 5 electrons per atom, possibly resulting from a mixture of the two configurations. We are planning a series of magnetic measurements which, we hope, will clarify the electron structure of the actinide metals in the monocarbide structure.

### 3. Thermodynamic Properties of Transition Metal Alloys (M. V. Nevitt, J. B. Darby, K. M. Myles)

A twin liquid-metal calorimeter for enthalpy measurements has been placed into operation at 415°C. After several minor modifications in design and mode of operation final calibration experiments were begun and are still under way.

The calibration is based on the heats of solution of pure metals in a liquid-metal solvent for which reliable values are available, specifically gold and silver in tin. Recent data indicate the precision to be + 2.5% or less rather than the value expected for this type of calorimeter, + 0.5%. The low precision arises primarily from a small change in thermal leakage induced by mechanical manipulations necessary to dispense a sample into the solvent. Modifications to insure constant thermal coupling between each calorimeter and its respective sample dispenser are now in progress. Experience to date suggests that the operation of a twin calorimeter in a vacuum is more difficult than in a gaseous environment because of the reduction in thermal coupling between adjacent components.

The vapor pressure of chromium over solid vanadium-chromium alloys has been measured by the torsion-effusion method in the temperature range 1450° to 1650°K. The computed chemical activities exhibit fairly small negative deviations from Raoult's law over the entire composition range. The excess free energies, the excess entropies and the enthalpies of formation have been calculated, and considered in terms of the changes in the characteristic properties of vanadium and chromium that occur upon alloying.

An unsuccessful attempt was made to extend the vapor pressure study to solid vanadium-manganese alloys as a sequel to the work on vanadium-chromium and vanadium-iron. In the temperature range where the partial pressure of manganese is within the range of the apparatus ( $10^{-3}$  to  $10^{-4}$  mm Hg), nonequilibrium conditions developed within the effusion cell because the diffusion rate of manganese is apparently lower than the effusion rate. A technique to circumvent this problem is being sought.

A similar study of solid-nickel-platinum alloys was performed for the nickel-rich alloys, but implausible vapor pressure results were encountered for the platinum-rich alloys. The spurious effect, which increased with platinum concentration, was thought to involve the entrance of some contaminant into the effusion cell at the experimental temperature. While the identity of the contaminant could not be established by chemical analyses, or by other means, an extensive series of remedial steps including baking out the vacuum system, elimination of sources of vapor contaminants, and the introduction of platinum getters around the effusion cell have reduced the effect to a tolerable limit, and the measurements are now being resumed.

Measurements of the vapor pressure of silver over solid silver-palladium alloys have been made. These data are currently being analyzed.

A drop calorimeter is now being assembled for the determination of heat capacities at elevated temperatures. The heat capacities will be used together with the free energy and enthalpy measurements to provide full elucidation of the thermodynamic properties.

4. Magnetic Susceptibilities and Thermoelectric Power Properties of Solid Solutions and Intermediate Phases (M. V. Nevitt, A. Aldred)

The study of magnetic susceptibility as a means of delineating the electronic structure of transition metal alloys has continued with measurements in the systems niobium-technetium, molybdenum-technetium, vanadium-technetium-aluminum, vanadium-iron, and vanadium-aluminum.

In alloys involving a neighboring transition metal solute in vanadium or niobium the rigid band approximation is a valid model in the body-centered cubic solid solution region. In many instances it has been possible to assess the contribution of s and d spin susceptibility to the total by empirically separating off the non-spin contributions. In such instances the spin susceptibility and its composition dependence are generally consistent with the density of electronic states at the Fermi surface as determined from low temperature specific heat. The effect of alloying seems to be an increase or decrease in the number of electrons in the band without affecting the form of the band.

This view is exemplified by results in the system molybdenum-technetium. The room temperature magnetic susceptibility increases from pure molybdenum ( $82.5 \times 10^{-6}$  emu/g-atom) to a small maximum ( $96.5 \times 10^{-6}$  emu/g-atom) at the equiatomic composition; further additions of technetium produce a decrease which reaches a minimum at 70 at.% Tc ( $\chi = 87.3 \times 10^{-6}$  emu/g-atom). Beyond this composition there is another increase to the value for pure technetium. No Curie or Curie-Weiss type of temperature dependence was observed in any alloy in the temperature range from 300°K to the superconducting transition temperature. The results indicate that the density of states at the Fermi surface increases upon initial addition of technetium to molybdenum and then decreases at technetium contents higher than the equiatomic composition, consistent with low temperature specific heat coefficients and superconducting transition temperatures in this alloy system.

In the system vanadium-aluminum, and in other systems in which a nontransition metal solute is involved, a rather different behavior is observed. The magnetic susceptibility decreases from  $5.63 \times 10^{-6}$  emu/g for pure vanadium to  $3.76 \times 10^{-6}$  emu/g for 35 at.% aluminum in vanadium. While the decrease in susceptibility with increasing solute concentration resembles qualitatively the behavior observed when transition metals dissolve in vanadium, it can be shown that most of the susceptibility arises from the orbital paramagnetism of the vanadium atom which is

essentially independent of composition. The orbital paramagnetism of aluminum is found to be zero; the aluminum acts simply as a diluent. The rigid band model is not applicable in this instance. When these data together with the measurements of low temperature specific heat and Knight shift are considered, it appears that the s-p electrons of aluminum have little or no interaction with the d electrons, which primarily determine the properties of the solvent. The outer electrons of aluminum are apparently not contributed to the vanadium d-band but instead constitute a low lying band, at the surface of which the wave functions are p-like.

Another approach to the study of the density of electronic states at the Fermi surface has been through measurements of thermoelectric power. Two apparently successful determinations have been made of the absolute thermoelectric power, S, for pure palladium. They agree with each other and with selected literature values to within 20%.

At high temperature, above the Debye temperature, the thermoelectric power is essentially due to the scattering of the electrons by lattice vibrations and may be expressed as:

$$S = - \frac{1}{3} \frac{\pi^2 k^2 T}{e} \left[ \frac{1}{N(E)} \frac{dN(E)}{dE} + \frac{1}{v^2} \frac{dv^2(E)}{dE} + \frac{1}{\tau} \frac{d\tau(E)}{dE} \right] (E = \zeta)$$

where k is Boltzmann's constant, T is the absolute temperature, e is the electronic charge, N(E) is the electronic density of states, E is the energy, v is the electron velocity,  $\tau$  is the relaxation time and  $\zeta$  is the energy at the Fermi level.

Therefore, the value of N(E) for palladium, determined from the low temperature specific heat, can be used with the free electron model to calculate S. At 700°C the calculated value of S is either -63 $\mu$ V/deg (if  $\tau$  is proportional to  $E^{3/2}$ ) or -21 $\mu$ V/deg (if  $\tau$  is assumed to be independent of E). These values bracket our experimental value, -42 $\mu$ V/deg, and we therefore have some encouragement for the use of the free electron model for our study of palladium-based alloys.

The alloy work in its present state, shows that when an element from groups lying to the left of palladium, specifically vanadium, chromium, manganese, iron, cobalt, tantalum or uranium, is dissolved in palladium there is in every case a decrease in S. The usual band model for palladium, due to Mott, would imply that S should first rise to a numerical maximum upon the addition of small amounts of these elements, and then decrease. It may be that we have not yet examined alloys sufficiently dilute to show the maximum. On the other hand, if the relaxation time is controlled by the density of states in the d-band, as has also been suggested, the controlling factor in the concentration dependence of S should be the slope of the d-band. In this case the solutes mentioned should cause S to decrease and then change sign. We intend to make measurements on more dilute alloys to clarify the ambiguity.

## 5. Ferromagnetism in Transition Metal Alloys (M. V. Nevitt, A. Aldred)

During the past eighteen months extensive changes have been made in the equipment used for measuring saturation magnetization. In earlier work on vanadium-iron and chromium-iron alloys it was found that the precision of the original ballistic technique was poor when the alloys being measured had weak magnetic moments. The first modification was a development and incorporation of an electronic integrator to measure the output of the detector coils. The integrator was expected to increase the precision of the measurement by about a factor of 5. However, when we attempted to use it for measurements at liquid helium temperature, we found that it was sensing a high level of noise in the detector coils, which had not been seen by the ballistic galvanometer used previously. The result was excessive scatter in the output signal. The noise was reduced by a factor of 10 by improving the stability of the magnet current, but an excessive signal-to-noise ratio remained. It was finally concluded that the noise was due to vibrations in the coils caused by translation of the specimen.

At this point it was decided to abandon the apparatus and employ the force method of measuring magnetization. This technique involves placing the specimen in a constant magnetic-field gradient and measuring the force exerted upon it. The new equipment which has been installed and placed in preliminary operation consists of a dual-sensitivity automatic recording vacuum balance mounted on top of a cryostat. The specimen is suspended in the cryostat in the gap between a pair of constant-gradient pole caps. The precision of this device should in principle be about five times better than that of the original induction method and the speed of measurement should be significantly increased. However, it is necessary that the magnetic field in the gap and its gradient be carefully mapped since it is intended that the measurements be absolute rather than comparative. In the latter case it would suffice to calibrate the gradient with specimens of known susceptibility. We believe that absolute measurements are a particularly important goal since a surprisingly small number of magnetization measurements have been made in this way.

When the apparatus is in satisfactory operation, we shall return to the measurements of the composition dependence of the magnetization of iron-base alloys in which the solute is either a nontransition element such as beryllium or gallium or a transition element such as molybdenum, technetium or tungsten.

## 6. Superconducting Transition Temperatures of Cr<sub>3</sub>O-Type Ternary Phases (S. T. Zegler and M. V. Nevitt)

The objective of this work is to elucidate the dependence of the superconducting properties of certain intermediate phases on crystallographic and electronic parameters. Initial work is being directed toward determining the superconducting transition temperatures of Cr<sub>3</sub>O-type ternary phases as influenced

by crystal lattice dimensions, valence electron concentration and atomic mass and volume.

Studies have been made of the occurrence of phases having the Cr<sub>3</sub>O-type structure in ternary alloys having the general composition V<sub>3</sub>(B,B') where B and B' are Fe, Co, Ni, Au, Rh, Ir, Si and Ga and also in Nb<sub>3</sub>(Rh,B) alloys where B is either Co, Ru, Pd, Os, Ir, Pt or Au. X-ray and metallographic data obtained for these alloys indicate the following:

1. Extensive mutual solubility can be expected between two A<sub>3</sub>B compounds which have the same A partner, and B partners that are members of the same or closely neighboring groups in the periodic table.
2. If the B partners are from widely separated groups, for example, in V<sub>3</sub>Co and V<sub>3</sub>Si, solubility may be limited.
3. Solubility of an element that does not form either a binary V<sub>3</sub>B or Nb<sub>3</sub>B phase is usually, but not always, extremely restricted in A<sub>3</sub>B compounds.
4. In most cases lattice parameters have the expected increase upon the substitution of a B partner having a larger atomic size. Exceptions to this rule occur, however, in the substitution of Fe or Co for Ni in V<sub>3</sub>Ni and of Co or Ru for Rh in Nb<sub>3</sub>Rh.

An apparatus has been constructed and calibrated for making inductive measurements of the superconducting transition temperature, T<sub>c</sub>, in nearly zero field in the temperature range 1.7 to 14.0°K. Measurements made on the Nb<sub>3</sub>(Rh,B) alloys indicate the following:

1. The T<sub>c</sub> for Nb<sub>3</sub>Rh is 2.52°K. The substitution of either Co, Ru, Os or Ir for 10% of the Rh atoms decreases T<sub>c</sub> while similar substitution of Pd has essentially no effect. The substitution of Ir has the largest effect decreasing T<sub>c</sub> to below 1.7°K. At greater substitutions of these elements T<sub>c</sub> is depressed further in all cases. In contrast Au and Pt substitutions increase T<sub>c</sub> to as high as 10.5°K and 9.8°K respectively.

2. The transition temperature of the alloys increases nearly linearly with increasing valence electron-to-atom ratio where all electrons outside of filled gas shells are considered as valence electrons. An even closer linear correlation is seen, however, between T<sub>c</sub> and the parameter  $\frac{e}{a} V^{-n}$ , where  $\frac{e}{a}$  is the electron-to-atom ratio, V is the volume of the unit cell, and n is a small integer.

#### 7. NMR Studies (D. Van Ostenburg, D. Lam)

NMR has proven to be a very useful technique for the study of the electronic and structural properties of materials. Our primary emphasis has been on metals, alloys, and intermetallic compounds.

It has been found for certain transition-transition metal alloys in their bcc region, e.g., V alloyed with other transition metals of the first and second long periods, that the Knight shift depends essentially on the electron/atom ratio rather than on the alloying species. These elements appear to conform to the rigid band model; that is, the number of electrons in the band of an element in the periodic table is simply increased or decreased by alloying with a neighboring element without appreciably affecting the band structure. On the other hand alloying V with nontransition elements, such as Al, led to the proposal that the constituents do not form a common conduction band but that the Al nuclei are electronically shielded from the rest of the matrix. The interpretation of the Knight shift data includes the partitioning of the Knight shift into portions associated with the s electrons, the d electrons, and the orbital paramagnetism. The alloy systems studied during the past year were the bcc region of vanadium-iron, vanadium-niobium, vanadium-aluminum, vanadium-technetium-aluminum, niobium-technetium, and the intermetallic compound  $\text{PuAl}_2$ .

Vanadium-Iron: The nmr parameters have been measured from 120 to 300°K and at various external fields. The Knight shift of  $\text{V}^{51}$  shows a maximum in the vicinity of 16 a/o Fe ( $e/a = 5.6$ ), while the line width increases slowly up to 20.2 a/o Fe and then rises rapidly at higher Fe contents. The nmr line widths increase linearly with frequency and are independent of temperature up to about 20 a/o Fe; at higher Fe concentrations they broaden at low temperatures. The fact that the nmr line width increases rapidly beyond 20 a/o Fe and increases at lower temperatures augments the determination of the composition where magnetic moments are first believed to appear. The Knight shifts of  $\text{V}^{51}$  in the nonmagnetic portion of this alloy system have been interpreted in terms of contributions from the Fermi contact term, core polarization and orbital paramagnetism.

Vanadium-Niobium: As remarked in the introduction, when V is alloyed with other transition metals a regularity is found in the data of the  $\text{V}^{51}$  Knight shift versus electron/atom ratio. That is, when  $K_V$  is plotted versus  $e/a$  for the alloy systems of V with Cr, Tc, and Fe, respectively, a maximum in  $K_V$  occurs near an  $e/a$  of 5.6. To gain further insight into this observation, a study of the  $\text{V}^{51}$  and  $\text{Nb}^{93}$  Knight shifts in the V-Nb bcc binary alloy system has been initiated. This is an alloy series where the  $e/a$  ratio is constant and where both nuclear species can be observed across the entire composition range; this work is in its early stages.

Vanadium-Aluminum Binary and Vanadium-Technetium-Aluminum Ternary Alloys: To explore further the concept of energy band compatibility among transition and non-transition elements, a study was made comparing the bcc region of the binary V-Al and ternary V-Tc-Al systems. For V-Al it was found that the  $\text{V}^{51}$  shift increased only slightly from 0.56% in pure V to 0.58% at 40 a/o Al in V, and that the change was nearly linear with Al content. The  $\text{Al}^{27}$  shift was negative and nearly independent of concentration within experimental error, with a value in the vicinity of -0.03%. This is to be contrasted with the Knight shift of pure Al which is +0.16%. The rigid band model is thought to be inapplicable to V-Al and similar systems. The

s-p electrons appear to have little or no interaction with the d electrons which primarily determine the properties of transition metals. The outer electrons of the Al are apparently not contributed to the vanadium d-band but instead constitute a low lying band, at the surface of which the wave functions are essentially p-like. For the ternary system the alloys were prepared by adding a fixed amount (5 a/o) of pure Al to requisite amounts of V and Tc. The compositions can be represented by the formula  $Al_5V_{95-x}Tc_x$  where x ranges from 0 to 50 a/o. Again the  $Al^{27}$  shift was found to be small. Compared with the values obtained on the V-Tc binary alloys, the shifts of  $V^{51}$  and  $Tc^{99}$  have the same magnitude and concentration dependence. The similar composition dependence of the  $V^{51}$  and  $Tc^{99}$  shifts in the binary and ternary alloys suggests that the electrons contributing to the shifts of  $V^{51}$  and  $Tc^{99}$  enter a common band, while the  $Al^{27}$  shifts, small in absolute magnitude and nearly independent of alloy composition with or without Tc, indicate that the Al conduction electrons are not contributed to the V-Tc d-band but again constitute a low lying band.

Niobium-Techetium: NMR measurements have been made on  $Nb^{93}$  and  $Tc^{99}$  across the bcc portion of this alloy system. In addition calculations<sup>(1)</sup> on the temperature variations of the electronic specific heats and magnetic susceptibilities have been made for Nb and Mo metals and Nb-Mo alloys using the density of states determined from low temperature specific heat data for 4d transition metals and their alloys. Temperature variations of the magnetic susceptibilities of these metals and their alloys are explained by including the temperature independent orbital paramagnetism and the effects of the negative (for Nb metal) and the positive (for the  $Nb_{0.75}Mo_{0.25}$  alloy) molecular fields. The Knight shifts of  $Nb^{93}$  and  $Tc^{99}$  in Nb-Tc and Nb-Mo alloys are shown to consist of contributions from conduction electrons of s-character, the exchange polarization effect, and orbital paramagnetism. The main contributions to these shifts appear to arise from the latter term.

Actinide Metals, Compounds and Alloys: To date the  $Pu^{239}$  nmr line has not been observed. Work will continue as more accurate nuclear magnetic moments are reported and the purity of the samples is improved.

One gram of neptunium oxide was received from Oak Ridge National Laboratory and investigated. The nuclear magnetic moment for  $Np^{237}$  is reported to be  $5 + 2.5$  nm. A search for the nmr absorption line was made over a range of magnetic moments ranging from 3.39 to 8.82 nm. No resonance was observed. One possible reason is that the line may have been broadened due to the large paramagnetism associated with this compound. Future work will continue when the pure metal is obtained. If the resonance is found it will provide a means for investigating alpha plutonium solid solutions since neptunium is the only element that dissolves to a large extent in alpha plutonium.

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(1) This work performed in conjunction with Drs. M. Shimizu and A. Katsuki of Nagoya University, Nagoya, Japan.

The Al<sup>27</sup> resonance line has recently been observed in the intermetallic compound PuAl<sub>2</sub>. The spectrum consists of a central line associated with the  $-\frac{1}{2} \rightarrow \frac{1}{2}$  transition and four satellites due to transitions among the levels associated with the Al<sup>27</sup> nuclear magnetic quantum numbers  $\pm \frac{3}{2}$  and  $\pm \frac{5}{2}$ . The satellite spacings are such as to yield a quadrupole coupling constant in the vicinity of 3.8 Mc. The central line width is composed of contributions from the second order quadrupole interaction, the anisotropic Knight shift, the dipolar interaction, etc. The study and analysis currently in progress should separate these contributions. When this information is complete the isostructural compound NpAl<sub>2</sub> will be examined and the results compared with that on UAl<sub>2</sub>. The composite data will be examined with the purpose of proposing possible models for the electronic structure of actinide metals and their compounds.

Spin-Lattice Relaxation: In order to exploit more fully the Knight shift data currently on hand and to study fluctuating internal fields in solids, a pulsed nmr spectrometer was designed and is nearing completion at this laboratory. During the past year, construction has advanced to the point where experiments can be performed at 8 Mc/sec.

Since our experiments are currently concerned with solid solutions and intermetallic compounds, where the absorption lines are usually broad, intense rf pulses are necessary. They are generated by gated rf high-power amplifiers. The energy contained in the pulses and the time intervals between pulses is controlled by changing the duration of the gate. The rf pulse is applied to the nuclear spin system by means of a transmitter coil and the nuclear induction signals are picked up by a receiver coil, which is orthogonal to the transmitter coil. The nuclear induction signals are coupled to the receiver and then displayed on an oscilloscope or fed into a box car integrator.

The unit is designed to operate at four frequencies, 4, 8, 13 and 18 Mc/sec with a maximum power output of 50 Kw. At present, the unit can be operated at 8 Mc/sec with the intended power output.

A dewar system has been constructed to provide temperatures from 4° to 300°K, with the specific requirement that samples could be introduced at low temperatures.

Tests of the unit at room temperature for V<sup>51</sup> and Al<sup>27</sup> in pure metals have been performed and the results are in good agreement with published data. Work in the V-Al binary system is currently in progress.

## C. Irradiation Effects in Metals and Alloys (T. H. Blewitt)

### 1. Transmission Electron Microscopy Studies of Radiation Effects in Thin Films (K. Merkle)

The studies on the energy dependence of fission fragment damage in single crystalline gold indicated that the primary knock-on atom has to receive an energy in excess of  $3 \times 10^4$  eV in order to initiate a displacement cascade that is large enough to result in a damage region which can be resolved by high magnification transmission electron microscopy. From the value of this threshold energy, the energy distribution of the primary recoils and the dose, one should then be able to calculate the density of spots in any given irradiation. The results obtained from irradiations with protons, deuterons, and alpha particles of various energies are in agreement with this picture. Present studies apply this to neutron damage.

Two theoretical models regarding fission track formation have been developed: the isolated particle model applies to films of isolated small metal or oxide particles. Another kind of track is observed in single crystalline insulators; here a cylindrical region of damage can be produced upon transfer of energy from the hot electrons to the lattice atoms. Present experiments are concerned with the influence of the substrate on track formation.

### 2. Irradiation and Solid Solution Strengthening Effects of Copper Single Crystals (T. J. Koppenaal)

The purpose of these studies is the investigation of the mechanism of strengthening in copper single crystals by neutron irradiation and/or solute additions. Thus far, it has been determined that aluminum additions to copper cause only a small enhancement of the room temperature strength after moderate neutron doses,  $\sim 10^{18}$  nvt or more. Experiments are being planned to investigate the temperature dependence of the yield strength. If the results show that the temperature dependence of the irradiation strengthening is solute independent (as the early results indicate), one must conclude that solutes do not affect obstacle formation on irradiation. We have, however, already observed a difference in the defect structure between pure copper and a Cu-14a/Al alloy; thus, not all defects are obstacles.

The largest effect of solutes appears to be that of lowering the activation energy at which the damage anneals out. This decrease in the activation energy is thought to be associated with the binding energy of either a vacancy-solute atom or an interstitial-solute atom.

### 3. Radiation Effects in Anisotropic Solids (B. Loomis)

The purpose of this research is the study of the effect of irradiation on anisotropic solids. The initial portion of the work has been the study of the

effects of annealing temperature on the volume changes of  $\beta$ -quenched uranium and uranium alloys containing krypton and xenon fission fragments. The work has been extended to include alpha recrystallized uranium with large and small grain sizes; preliminary results indicate a substantial effect of grain size on the volume change.

Observations of the microstructure utilizing electron microscopy techniques will also be made to aid the interpretation of the results. Irradiation-induced growth will be studied utilizing the low temperature facility in the CP-5 reactor. In these experiments growth will be investigated in fissile materials, such as uranium and uranium-doped zirconium and in nonfissile anisotropic materials, such as zinc, bismuth and magnesium. In the latter case energetic neutrons will be used as the bombarding particle. The growth of the specimens will be determined by a direct measurement of the length changes in various crystallographic directions.

To aid the understanding of the growth, specimens suitable for electron microscopy examination and measurements of the change in lattice parameters will also be irradiated.

#### 4. Pores in Solids (E. Gruber)

This program is concerned with the behavior of fission gas bubbles in solids. Theoretical consideration has been given to the problem of migration of these bubbles under the influence of a thermal gradient. This migration appears to occur primarily by diffusion of the matrix atoms over the inner surface of the bubble. Appropriate expressions have been derived to express the bubble diffusivity and bubble velocity in the presence of a driving force, such as a thermal gradient.

The results are being used to predict coalescence behavior of bubbles by consideration of the bubble size distribution and the change in this distribution with annealing time. The approach employs finite difference methods and the calculations are being made by means of the CDC 3600 digital computer.

This theoretical work will be augmented in the near future by experimental work which will include electron microscope observations of bubble migration and swelling measurements on postirradiation annealed specimens. The affect of a thermal gradient on swelling is of particular interest.

#### 5. Experimental and Theoretical Studies of the Formation and Annihilation of Point Defect Clusters in Pure and Impure Metals (R. M. Cotterill)

The theoretical work involves: a) A calculation of the time dependence of the concentration of various defect clusters (divacancies, trivacancies, etc.) during quenching and subsequent annealing. These calculations can be applied to both pure and impure metals, and, with a slight modification, the program is applicable to the case of an irradiated metal. b) Calculations of the binding energies of various defect clusters. These calculations involve use of either a Morse potential or a Born-Meyer potential. Relaxations of surrounding atoms are taken into account

but no allowance is made for electron redistribution. The results of this study will later be used in (a).

Of the two types of experiment, the more straightforward involves irradiation of previously-annealed specimens. An example of this type is the experiment in which pure copper and Cu-14a/oAl were neutron-irradiated under identical conditions. The pure copper was found to contain both the small vacancy clusters and the larger interstitial loops normally observed in this metal. The alloy contained only the vacancy clusters. This result is taken as evidence of interstitial-solute cohesion in the alloy. Other alloy systems are now being examined. This type of experiment is being repeated at 78°K for 40 MeV  $\alpha$ -irradiation in the cyclotron. The other type of experiment exploits the effect observed by Cotterill and Jones in which clusters of vacancies, introduced by quenching, are annihilated during  $\alpha$ -irradiation (presumably by the interstitials that are generated during irradiation). It has now been established that neutron irradiation produces the same result. An interesting side effect is also observed. Interstitial loops are not formed in the previously-quenched specimen because all the interstitials are lost at the original vacancy clusters. This type of experiment is also to be carried out at 78°K in an electron microscope and at 4°K in the CP-5 Reactor.

#### 6. Effect on Neutron Irradiation on the Precipitation Process (J. Horak)

The purpose of this research is to investigate the effects of irradiation-induced defects on the precipitation process. Present experiments involve the study of aluminum base Al-Cu, Al-Zn, Al-Mg, and Al-Ag alloys in the as-quenched condition and the Al-Cu and Al-Zn alloys in the reverted condition. The 4.2°K irradiations are followed resistometrically as are the subsequent isochronal anneals to room temperature. These measurements will be followed by small angle X-ray scattering to determine the size and number of precipitation nuclei present in irradiated versus unirradiated material. Alloy compositions well below those where precipitation is normally detected are also being studied to provide information on the nature and extent of the solute atom-point defect interactions.

#### 7. Determination of Lattice Parameter Changes in Metals Arising from Irradiation and Its Subsequent Recovery (B. D. Sharma)

One of the most important questions remaining to be answered in the field of irradiation damage is the migration energy of vacant lattice sites and interstitial atoms in copper. This point is a key one to a basic understanding of the mechanism of irradiation damage. In this experiment when the recovery of irradiation damage is followed by the measurement of electrical resistivity and lattice parameter, the question can be answered. This is true as the vacant lattice sites will cause a decrease in lattice parameter, whereas the interstitial atoms will cause an increase in lattice parameter. If a fraction of the defects, as current experiments seem to indicate, reach a surface of the metal without being annihilated by meeting one of their opposite number, then the lattice parameter will change at a rate which is either too fast or too slow for a rate based on complete annihilation.

A plot of lattice parameter change against that of electrical resistivity will show such a deviation, and it should be possible to delineate between the motion of interstitial-type defects and vacant lattice site defects.

This experiment is currently being undertaken and the in-pile cryostat is now under construction. A precision X-ray diffractometer is presently being prepared. Results are expected from this experiment within next year.

8. Determination of Energy Release Associated with the Recovery of Irradiation Damage (M. Lucas)

One of the most important pieces of information to be attained in the study of irradiation damage is the amount of energy release associated with the recovery process. This information is particularly useful as the formation energy of vacancies and interstitials are rather well known.

Currently measurements have been made by two independent investigators but the results differ by a factor of two. An experiment is under way to repeat these measurements and obtain a more accurate figure of the energy release during the recovery of irradiated metals.

It is believed that greater precision can be reached than in the past as it is possible to bombard in a higher neutron dose than was the case in the previous experiments.

D. X-ray and Neutron Diffraction Studies (S. S. Sidhu)

1. Neutron Diffraction Instrumentation (M. Mueller)

In our investigation of the crystal structure of alpha uranium at low temperature we have previously indicated that it is necessary to use a longer wavelength neutron beam and also to carefully exclude the  $\lambda/2$  component. We have found that a germanium monochromator satisfies both of these objectives. It was found that sufficient imperfections could best be introduced in the germanium crystal by a small compression at elevated temperatures.

2. Neutron Coherent Scattering Amplitudes (L. Heaton, M. Mueller)

Since neutron scattering amplitudes can only be determined experimentally, a continuing effort is made to obtain coherent scattering measurements on isotopes as they become available as well as improving previously reported values. The following were determined in the usual way and were presented orally at the International Conference on Nuclear Physics with Reactor Neutrons.

<u>Atomic Number</u>	<u>Element or Isotope</u>	<u>b (10<sup>-12</sup> cm)</u>
12	Mg	0.475
19	K	0.34
	K <sup>39</sup>	0.37
37	Rb	0.85
	Rb	0.83
40	Zr	0.70
43	Tc <sup>99</sup>	0.68

### 3. Crystal Structure of Ti<sub>2</sub>Cu, Ti<sub>2</sub>Ni, Ti<sub>4</sub>Ni<sub>2</sub>O and Ti<sub>4</sub>Cu<sub>2</sub>O (M. Mueller)

Lattice constants were determined for all four phases using X-ray powder diffraction films. Atom positional parameters of all four phases have been determined from observed neutron intensities. X-ray diffraction calculated intensity data has also been presented for Ti<sub>2</sub>Cu to point out the particular suitability of neutron diffraction in spite of the large unit cell size. Interatomic distances have been determined using the positional parameters obtained from neutron diffraction.

### 4. Structure of Disodium Tetranitritonitrosohydroxyruthenate (III) 2-Hydrate (M. Mueller)

The determination of the crystal structure of this compound by neutron diffraction has been completed. We have refined the positional parameters of all 16 atoms together with anisotropic temperature factors for each, and have calculated the resulting RMS thermal displacement of each atom.

The structure can be envisioned as consisting mainly of 6-fold coordination about three separate atoms; namely the Ru, Na<sub>1</sub> and Na<sub>2</sub>, thus forming three different kinds of octahedra which include almost all of the atoms within the structure. The Ru octahedron has four nitrogens from the NO<sub>2</sub> groups, a nitrogen from the NO group, and an oxygen from the OH group. Both Na<sub>1</sub> and Na<sub>2</sub> have six oxygens about each, which are from the NO<sub>2</sub> groups, OH groups or the H<sub>2</sub>O. By the use of this description it is evident that these octahedra form an interlocking chain throughout the structure in which there are common atoms or common edges shared between octahedra. Each of the three octahedrons are oriented relatively the same in the unit cell. Four atoms in each are arranged in a near coplanar square in which this plane is perpendicular or nearly so to the mirror plane (or parallel to the b axis). The other two atoms involved in each of the 6-fold coordination lie along a line perpendicular or nearly perpendicular to this square plane, thus forming the octahedra.

This octahedral arrangement leaves no octahedrons dangling but rather they are all tied to each other. The only atoms not included in these octahedra are the hydrogen of the OH groups, the oxygen of the NO group, the hydrogens of the H<sub>2</sub>O, and the O<sub>3</sub> and O<sub>6</sub> of the NO<sub>2</sub> group. From the distance involved between the O-H . . . O it is evident that there is little or no hydrogen bonding. The distances and angles found in the H<sub>2</sub>O part of the structure seem reasonable.

5. Structure Determination of Uranyl Nitrate Hexahydrate, UO<sub>2</sub>(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O (M. Mueller, J. C. Taylor)

Suitable crystals of this compound have been grown and the collection of three-dimensional neutron diffraction data are under way. Whereas early X-ray results indicated that the crystal was orthorhombic, space group Cmc<sub>2</sub>m, a later piezoelectric study and two X-ray investigations proposed a noncentrosymmetric group Cmc<sub>2</sub>1. Two recent infra-red investigations are in conflict with regard to the ionic or covalent bonding of the NO<sub>3</sub> groups. The first of the above X-ray investigations has indicated an ionic compound composed of [UO<sub>2</sub>(H<sub>2</sub>O)<sub>6</sub>]<sup>2+</sup> and [NO<sub>3</sub>]<sup>-</sup> ions with the six water molecules in the form of a hexagon around the uranium, whereas later X-ray study has suggested a nonionic structure with the uranium coordinated to two NO<sub>3</sub> groups and two H<sub>2</sub>O, with the other four H<sub>2</sub>O loosely held. It is planned to use neutron data to resolve the above conflicts as well as locate the hydrogens of which there are a number in the structure. A parallel X-ray investigation is to be carried out by Prof. Lynton in British Columbia.

6. Chemical and Magnetic Order in PtMn<sub>3</sub> (S. S. Sidhu)

The susceptibility-temperature measurements of PtMn<sub>3</sub> in the room to 250°C temperature range show an anomaly, which, as shown by X-ray diffraction measurements, does not result from a phase change of the alloy. A neutron and X-ray diffraction study was made of the chemical and magnetic order in the above temperature range to explain this anomaly, and is being extended to cover a larger temperature range to determine the main characteristic of the magnetic behavior of the alloy and its dependence on the chemical order and disorder.

The crystalline structure of the PtMn<sub>3</sub> alloy is face-centered cubic with four atoms per unit cell and a<sub>0</sub> = 3.84Å. The structure factor for the disordered state is:

$$\left| F_{hkl} \right| = \left( \frac{b_{Pt} + 3b_{Mn}}{4} \right) \left\{ 1 + e^{\pi i(h+k)} + e^{\pi i(h+l)} + e^{\pi i(k+l)} \right\} \quad (1)$$

and for the ordered state, in which, say, Pt is at: 0 0 0, and 3 Mn at: 1/2 1/2 0; 1/2 0 1/2; 0 1/2 1/2,

$$\left| F_{hkl} \right| = b_{Pt} + b_{Mn} \left\{ e^{\pi i(h+k)} + e^{\pi i(h+l)} + e^{\pi i(k+l)} \right\} \quad (2)$$

where  $b_{Pt}$  and  $b_{Mn}$  are coherent nuclear scattering amplitudes for Pt and Mn respectively. The above expressions are also applicable to X-ray structure factors in which  $b_{Pt}$  and  $b_{Mn}$  are replaced by X-ray scattering factors  $f_{Pt}$  and  $f_{Mn}$  respectively. Neutron and X-ray structure factors squared are given in Table I.

Table I. Structure Factor Squared for  $PtMn_3$

State	Miller Indices	X-rays		Neutrons	
		$F_{hkl}^2$	$F_{hkl}^2$	$F_{hkl}^2$	$\times 10^{24} \text{ cm}^2$
Disordered	(a) $hkl$ all odd or all even	$(f_{Pt} + 3f_{Mn})^2$			0.0237
	(b) $hkl$ mixed	0			0
Ordered	(a) $hkl$ all odd or all even	$(f_{Pt} + 3f_{Mn})^2$			0.0237
	(b) $hkl$ mixed	$(f_{Pt} - f_{Mn})^2$			1.7371

$$b_{Pt} = 0.95 \times 10^{-12} \text{ cm}; \quad b_{Mn} = -0.368 \times 10^{-12} \text{ cm}.$$

It is apparent from the structure factor squared values that while X-ray diffraction patterns of the disordered and the ordered alloy would give normal reflections for this type of structure, neutron diffraction patterns would be unique. This is confirmed by the patterns obtained. A neutron diffraction pattern of the ordered alloy consisted mostly of mixed Miller indices reflections. Practically no diffraction peaks were observed for the all odd or all even Miller indices planes. This uniqueness is found in the neutron diffraction patterns of the face-centered cubic nuclear null-matrices in which the atoms making up a null-matrix transform to ordered positions.

The neutron diffraction patterns of the ordered alloy made at room temperature and at 250°C showed that the crystallographic structure of the alloy was the same at both temperatures, but there were marked differences in the relative intensities of (100) and (110) reflections at the two temperatures. These differences are ascribed to superposition of magnetic intensity on nuclear intensity, the magnetic intensity resulting from alignment of magnetic moments at room temperature. The alignment and disalignment of magnetic moments in this temperature range account for the reported anomaly in the susceptibility-temperature curve of the alloy.

## 7. The Scattering of Neutrons by Liquid Alloys of Sodium and Cesium (L. Heaton)

Neutron diffraction patterns have been obtained and inverted to atomic radial distribution curves for liquid alloys of sodium and cesium of six different compositions over a temperature range from the alloy's melting point to 365°C. The alloys were contained in hermetically-sealed cylindrical cells of vanadium of one cm diameter and five cm in length. The excellent corrosion resistance of the vanadium to the alloys avoided sample contamination and the vanadium's negligible scattering amplitude gave no spurious peaks.

The atomic radial distribution curves show nondiscrete first peaks. While these data do not preclude the existence of weakly bound molecules or clusters with atomic distances nearly the same as distances between neighboring free atoms, the distribution curves do show that no permanent compact molecules exist in the liquid sodium-cesium system. The radial distribution curves of each alloy except in the vicinity of 80 a/o sodium have the general shape and behavior exhibited by the monatomic elements themselves in that there is a small increase of nearest neighbor distance and an appreciable decrease in number of nearest neighbors with temperature. Samples of 78.7 a/o sodium and 83.4 a/o sodium gave distribution curves of which the first peaks are broad, though not diffuse, with plateau-like tops at all temperatures.

## 8. Crystallographic Computer Programs (M. Mueller, L. Heaton, S. S. Sidhu)

Since the Laboratory has now obtained a CDC 3600 computer we are in the process of converting our crystallographic computer programs so that they can be used in this computer with a free flow of the input and output data. This will require programs for (1) generating a complete set of  $hkl$ 's appropriate for the crystal together with the angle settings for obtaining the data on the automatic Neutron Diffractometer I (2) processing the output data and (3) permitting this output data to be used as input for a number of programs, such as, least squares, superposition and Fourier programs for the analysis of the crystal structures. This will require the rewriting of some programs so as to be suitable for CDC 3600 operation as well as the writing of new programs, both to be carried out in cooperation with the Applied Mathematics Division.

## E. Corrosion Research (J. E. Draley)

### 1. Electron Optical Study of Surface Reaction Products (R. Hart)

One important aspect of metallic corrosion and oxidation involves knowledge of physical attributes of the metal and structural relationship between these and the overlying reaction product. Thus a detailed knowledge of the physical relationship between metal and compound(s) by itself and more importantly tied in with other investigations such as kinetic studies and electrochemical or chemical behavior will lead to a better understanding of the problem.

The Al-steam system has proved to be particularly interesting in the study of morphology and structural relationships between metal and corrosion product.

In steam at temperatures above 600°C and pressures up to 1000 psi aluminum is filmed with a thin, highly protective oxide, namely  $\gamma\text{-Al}_2\text{O}_3$ . The morphology of these films is well-defined in electron micrographs and their orientations are directly related to the grain orientations in the underlying metal.

There are other temperature and pressure ranges where aluminum is not nearly as corrosion resistant to steam. For instance, just above the critical temperature of water (374°C) aluminum will rapidly disintegrate. The product consists of  $\alpha\text{-Al}_2\text{O}_3$  (corundum) and  $\gamma\text{-Al}_2\text{O}_3$ , the relative proportions of these two oxides varying from sample to sample.

Available data indicate that  $\alpha\text{-Al}_2\text{O}_3$  should not form under these conditions and experiments are in progress to investigate this system more closely.

## 2. Oxidation of Zirconium (D. Bradhurst, J. E. Draley)

The objective is to determine the mechanism by which a solid product limits reaction between a metal and a gas. Many features of this mechanism are not understood, in particular for metals such as zirconium. These include the cubic law of oxidation, transitions from one rate law to another and the dependence of this behavior on the presence of water vapor. By closely relating the EMF which develops across the growing oxide scale on zirconium and its structural features, the growth mechanism can be identified.

Measurements of the EMF across the scale forming on zirconium in oxygen have indicated that the oxidation is controlled both by ionic and electronic conduction. By using this EMF, and the measured resistance of the growing scale, it is possible to estimate the free energy change in dissolving oxygen in the (anion-deficient)  $\text{ZrO}_2$ . From this and  $\text{O}_2\text{-ZrO}_{2-x}$  equilibrium measurements it should be feasible to estimate the defect structure in the growing oxide.

Application of a more negative (than normal) potential to the metal with respect to the external oxide surface causes a reduction in oxidation rate. Similarly, a more positive potential increases the oxidation rate. The analogy to aqueous systems suggests an investigation of the polarization behavior of zirconium in oxygen.

During oxidation, zirconium oxide is observed to crack. Experiments allow estimates of the stress levels in the oxide film, and an attempt is being made to correlate mechanical properties of growing oxide with oxidation behavior.

### 3. The Kinetics of Aqueous Aluminum Corrosion (S. Mori, J. E. Draley)

The chemical and physical aspects of corrosion are being studied as a means of determining the mechanisms of the corrosion of aluminum in water. The presence of oxide films and the local nature of the reaction indicate that rate control is related to local degradation and repair of corrosion product oxide. Determination of the amount of metal corroded, the weight of the adherent corrosion product, and the amount of product lost to the water permits calculation of the composition of the corrosion product coating.

Careful measurements have shown that during two periods the amount of corrosion of "commercially pure" aluminum varies with the logarithm of time. Between these two periods, there is a break upward in the corrosion curve. The logarithmic behavior has been interpreted in terms of alternate film growth and breakdown, with the latter perhaps induced by the accumulation of corrosion product hydrogen beneath the protective film. The effects of external parameters such as temperature and oxygen content of the water on film growth rates and the breakdown process are being studied to allow examination of reaction mechanisms.

### 4. The Aqueous Corrosion of Aluminum Alloys at Elevated Temperatures (J. E. Draley W. Ruther)

The use of rapidly flowing water as a corrodent is proving to be a valuable tool in elucidating the mechanism of aluminum corrosion at elevated temperatures. Environmental effects, which are either absent or lost in the experimental errors in static water, become very important in dynamic corrosion. Explaining these effects should provide a better general understanding of the interactions at the water-aluminum oxide interface during corrosion.

Corrosion tests have been completed in which different aluminum alloy systems, oxygen levels, analyses of flowing stream solids, surface areas, flowing path length and changes in stream temperatures have been variables. From the results of these tests it has been tentatively postulated that precipitation and adherence of a colloid (usually but not always a form of aluminum oxide) on the outer surface of the protective oxide film is essential to a low aluminum corrosion rate.

The source of the colloid is assumed to be the neutralization of alkaline (or acid) streams (carrying the aluminum in a soluble form) issuing from cracks and fissures in the protective oxide. This mechanism seems to have validity for the corrosion of aluminum under other conditions as well.

In current tests, buffers are being used to prevent large pH changes in the fissures, and thus to influence corrosion behavior.

### 5. Polarization Studies (R. Legault, J. E. Draley)

Since the processes occurring during aqueous corrosion involve the transfer of charge, the interrelationships between overall current flowing, the potential,

and the corrosion rate allow the deduction of the important steps in the corrosion reaction. Variation of the basic parameters while making the measurements should make it possible to deduce the roles of the various processes in controlling corrosion.

Methods of measurement have been developed and polarization curves have been determined for almost 20 pure metals in boiling distilled water. Current research will determine whether normal impurities in the water have significant influence on the electrochemical processes occurring on aluminum. It should then be possible to examine polarization data from the point of view of learning important factors in the growth and breakdown of protective films.

## F. Ceramic Materials Research

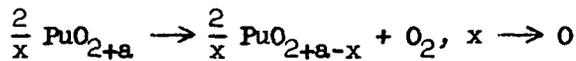
### 1. Dislocations and Irradiation-Induced Defects in Oxides (P. Stablein)

In our previous work we concentrated on the study of neutron irradiated MgO single crystals in which the interaction of dislocations with irradiation-induced defects was studied through dislocation etching techniques on samples deformed by bending and by hardness indentations. Analyses of these in conjunction with slip line traces were made to determine dislocation generating stresses and dislocation movement stresses and their behavior and how they change during annealing. This work has been extended to fission fragment and deuteron bombardments. Crystals whose thickness is larger than the deuteron range are being studied. The hardening produced by the deuteron itself when it stops in the lattice is greater than that caused by the damage produced in passing through the lattice.

Studies on the dose dependence and the energy dependence of the bombarding particle on the mechanical properties of MgO are in progress. We plan to extend this study to include other crystals, such as TiO<sub>2</sub> and CoO, which exhibit non-stoichiometry so that excess vacancies can be present for interstitial annihilation. As an adjunct to this research, single crystal growth studies on oxides are also under way.

### 2. Defect Equilibria in PuO<sub>2</sub> (L. Atlas)

At temperatures above 600° or 700°C, the fluorite structure of PuO<sub>2</sub> can apparently vary in composition between about PuO<sub>1.62</sub> and PuO<sub>2.00</sub> - possibly even up to PuO<sub>2.09</sub>. Defect equilibria, including the free energy, enthalpy, and entropy of the general reaction



are being investigated. Experimental methods include:

1. An electrochemical cell using a stabilized zirconia electrolyte,
2. measurements of electrical conductivity as a function of temperature and the partial pressure of oxygen,
3. measurements of oxygen dissociation from  $\text{PuO}_{2+a}$  using a thermal conductivity gas analysis system.

In addition to the thermodynamic data listed above, it is hoped that this combination of techniques will provide information on (a) the type of defects present, (b) the equilibrium constants for their formation and dissociation, and (c) the energies involved in these processes. At the present time test experiments are being carried out with  $\text{TiO}_2$ .

### 3. Effect of Surface Structure Upon the Catalytic Activities of Solid Oxides (M. Volpe)

The purpose of this research is to determine the relative importance of the various crystalline structural factors on the catalytic activity of solid oxides. The general approach is that of measuring the catalysis rate of some chemically simple gaseous reaction on exposed crystallographic faces of single crystals having different point and line defect concentrations and different degrees of surface roughness.

The choice of a suitable reaction for these studies was dictated by a desire for chemical simplicity and by the availability of the oxides in the form of large single crystals. The decomposition of nitrous oxide on MgO or on MgO-CoO solid solution ( $\text{N}_2\text{O} \rightarrow \text{N}_2 + 1/2 \text{O}_2$ ) was chosen to start this investigation.

The apparatus has been designed, constructed and tested out. It has been found possible to measure the rate of decomposition of nitrous oxide on one single crystal wafer of CoO-MgO (50 mole % CoO) having the dimensions, 1 cm x 0.5 cm x 0.05 cm. There is some interference due to catalysis by the walls, but certain apparatus modifications have been made to reduce this wall reaction to a negligible amount. The modified equipment has just now been put into operation.

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**Contractor:** Argonne National Laboratory, Argonne, Illinois

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**Contract Title:** PHYSICAL RESEARCH IN THE SOLID STATE SCIENCE DIVISION

**Investigators:** O. C. Simpson, Director, Solid State Science Division and staff

**Scope of Work:**

The general aim of the research program in the Solid State Science Division is the basic understanding of the properties of solid materials and of their interactions with various environments. Emphasis is frequently placed on the interaction itself or on the result of the interaction as in the case of radiation damage studies. In other cases, the interaction of radiation fields or other environments (very slow neutrons, high magnetic fields, microwaves, light, gamma rays and x-rays, sound, low and high temperatures, etc.) are used as indispensable experimental aids in the study of the properties of solid materials both in the nominally perfect condition or after exposure to more severe environmental situations. Many materials of particular significance to nuclear energy and related projects are specifically studied such as graphite, uranium sulfide and other actinide compounds, ice and a few additional hydrogen bonded materials, rare earth metals, etc.; however, the work also includes many other materials that readily lend themselves to studies which serve to elucidate the general features of atomic and electronic structure and properties of crystalline materials and the role of defects in determining their properties.

A. Application of Resonance Effects to the Study of Solids

1. Optical and Spin Resonance Properties of Single Crystals - Color Center Research

C. J. Delbecq, J. Gabriel, D. Schoemaker, J. Sierro, S. Susman, E. Yasaitis, P. Yuster

Studies of the optical absorption and of the paramagnetic resonance absorption properties of irradiated alkali halide single crystals prepared with controlled impurities have revealed many interesting and important aspects of radiation induced defects in these materials. The

purpose of the investigations is to determine the characteristics and interrelations of defect centers. The data, concepts, and ideas developed in the studies are very useful in the general radiation field. Certain selected projects now in progress are as follows:

The nature of the afterglow and the thermoluminescent properties of x-irradiated KCl-Ag and KCl-Tl crystals are being studied. Further ESR measurements, particularly on KCl-Tl, are being made in an attempt to identify and characterize the electron and hole traps and to determine their roles in the luminescent behavior.

The relationships of the  $V_1$ -center in KCl and the  $FCl^-$  center in KCl are being studied with the aim of obtaining information on the mechanism of production of vacancy-interstitial pairs in the alkali halides. Related studies are in progress to determine the role that impurities play on interstitial formation since it has been found that  $Na^+$  enhances the rate of production of  $V_1$ -centers considerably.

ESR measurements on low temperature x-irradiated KCl-KBr single crystals have revealed that under certain conditions a new type of  $ClBr^-$  mixed center is formed lying in a [001] plane but with its molecular axis  $11.7^\circ$  off of the [110] direction. Further ESR and optical work are required to develop a better understanding of this defect center. Optical and ESR studies are also being carried out on mixed KCl- $Na_2S$  single crystals and on natural fluorite,  $CaF_2$ , to determine the nature of the color centers in these materials.

The Laboratory's new high intensity pulsed Van de Graaff generator will be used for fast transient studies of color centers. With this generator, it should be possible to create a large number of F-centers in excited states. With the use of a flash lamp, spectrograph and photographic plates it may be possible to obtain for the first time the absorption spectrum of the excited state of the F-center. Other centers having comparable or longer lifetimes may also be studied in the same fashion.

Pure, single crystalline KCN was prepared by a zone melt procedure, and the color centers produced in this material, which has the alkali halide structure, have been studied. Color centers analogous to the F- and M-centers in alkali halides are formed; however, a major difference has been found in the crystal field splitting.

A versatile high field spin resonance spectrometer has been under construction. Experiments to study thallium<sup>+</sup> and thallium<sup>++</sup> impurities and H-centers in alkali halides are planned. The apparatus will also be used to investigate unexplained lines in the spectrum of  $V^{++}$  in NaCl and for molecular ions analogous to  $FCl^-$ .

## 2. Electron and Nuclear Magnetic Resonance Studies

Electron and nuclear resonance techniques have been invaluable aids in the detection of radiation effects in materials and in the study of crystalline field effects.

a. Electron Spin Resonance

E. Avery, I. Brown, B. Smaller

An important phase in the radiation damage process in biological and chemical systems is that of the transfer of energy between similar and dissimilar molecules. Investigations of the triplet state produced in rigid (glassy) media are in progress to better understand the migration of energy between acceptors and donors and the transfer of triplet excitation with rearrangement of spin state.

A standard pulse height analyzer has been adapted to sort short-lived signals from an EPR spectrometer from accompanying "noise". This recent development will be used to study short-lived free radicals and metastable states produced by pulsed electron irradiation.

b. Nuclear Magnetic Resonance of Stable or Long-Lived Nuclides

D. O'Reilly, G. Schacher, T. Tsang

Measurements of Knight shifts of alkali metal and  $N^{14}$  nuclei in metal ammonia solutions are nearly complete. New concepts regarding the interaction of the unpaired electrons with the alkali metal ions have emerged from a comparison of this experiment and the theoretical model. The work on metal-ammonia solutions is related to the study of electron-electron interactions in solid state physics and has aspects related to the radiation chemistry of liquids such as water.

Studies of ferroelectric materials by resonance techniques are in progress. Measurements of the  $O^{17}$  resonance in  $CoO$  and  $MnO$  and the  $F^{19}$  resonance in  $KCoF_3$  at various temperatures have been interpreted to yield the unpaired electron spin densities in the oxygen and fluorine 2s orbitals.

c. Nuclear Magnetic Resonance of Short-Lived Nuclides

D. Connor and D. Davis

A novel technique has been developed at Argonne to study the nuclear magnetic resonance of nuclides which are too short-lived for investigation by conventional methods. This technique uses the anisotropy in  $\beta$ -emission as the means of detecting and measuring nuclear polarization. The nuclear moments of  $Li^6$  (0.85 sec) and  $F^{20}$  (11 sec) have been determined with the  $LiF$  sample at room temperature;  $B^{12}$  (.02 sec) is now under study with the sample at  $77^\circ K$ . A cryostat suitable for use in the liquid helium region is under development. Such equipment should make it possible to study several other short-lived nuclei by this technique and may provide a unique microscopic probe for radiation effects studies since the magnetic relaxation time is a function of the crystalline environment.

### 3. Solid State Mössbauer Experiments

C. Kimball and J. Mullen

Structure-related magnetic and electronic properties of transition metal alloys are under investigation using nuclear resonance fluorescence. Isomer shifts at  $Fe^{57}$  in V-rich V-Fe alloys have been measured for alloys of 7 to 30% Fe.

Mössbauer spectra of iron in intermetallic compounds of the  $\alpha$ -manganese structure are being examined as a function of temperature to further elucidate the behavior of the isomer shift and the hyperfine field with a change in the crystal site and alloying element above and below the antiferromagnetic ordering temperatures.

A study has been completed of the charge state and environments of  $Fe^{57}$  ions in NaCl using the Mössbauer effect as a microscopic probe to measure internal crystalline fields and electronic charge densities at the  $Fe^{57}$  nuclei. The technique proved to be very satisfactory and will be applied from time to time to similar problems with other systems.

#### B. Experimental Studies of Material Classes

##### 1. The Physical and Chemical Properties of Graphite

M. Dzurus, G. Hennig, and G. Montet

The objective of this work is to increase the basic understanding of the solid state physics and chemistry of crystalline carbon, especially graphite. Radiation damage and chemical reactivity studies are made on both natural single crystals and polycrystalline nuclear reactor-grade graphite.

A new technique of "decorating" cleaved surfaces of graphite with gold and subsequent examination in the electron microscope has been developed and successfully used to distinguish between interstitial atoms and lattice vacancies. The method is also being used to determine vacancy energies, displacement energies, and diffusion constants in graphite.

Surface atoms of graphite have been displaced by bombarding the crystals with argon ions of known energy using a low energy bombardment source originally developed for studying displacement effects in metals. Preliminary results indicate that the displacement energy of surface atoms is between 35 and 45 eV.

A technique has been developed using the chemical reactivity of ozone and graphite to "peel" single crystal graphite samples atomic layer by atomic layer. The method is being used to study radiation effects in graphite. Reaction with ozone permits complete removal of one single layer plane of graphite at a time. Surface reactions with other materials such as atomic hydrogen and halogens are also studied.

An improved method of autoradiography is being developed which, it is hoped, should permit a resolution of several hundred angstroms in the detection of the position of injected radioactive foreign atoms in graphite crystals.

## 2. Electrical and Magnetic Properties of Cubic Actinide Compounds

M. Kanter

Galvanomagnetic measurements on polycrystalline samples of uranium monosulfide have shown it to be ferromagnetic with a spontaneous moment of about one Bohr magneton per atom and a Curie point at 178-180°K. The compound has been found to have electrical properties of a semi-metal with predominant conductivity by positive carriers. A preliminary band model has been postulated based on two overlapping bands.

The work will be extended to measurements of thorium sulfide, uranium phosphide, and their solid solutions with US in an effort to confirm the band structure which has been postulated. Other compounds such as UC, UN, UAs, and UTe may also be investigated as suitable samples become available. The work is coordinated with other work at the Laboratory on phase studies, heat capacities, and thermoelectric properties in order to lead to a comprehensive understanding of these compounds which have a potential use as fuels in advanced reactors.

## 3. Low Temperature Radiation Effects in Hydrogen Bonded Compounds

J. McMillan

Work in progress covers the study of low-temperature states of aggregation of hydrogen-bonded compounds, water, hydrogen-peroxide, hydrazine, alcohols and amines, from the view of their thermal behavior (nucleation and crystal growth) and interaction with ionizing radiation. The magnetic characteristics of the trapped radicals produced by irradiation are affected by the nature of the matrix (glass or crystal) and the kinetics of recombination shows some correlation with the thermal behavior during warmup. Large doses of irradiation (several hundred million roentgen) lead to damage saturation whose value depends on the temperature. It is intended to determine whether or not this value depends on the type of aggregation. The techniques used in these studies are electron spin resonance and thermal analysis. This work is closely related with interstellar radiation chemistry and with the storage in outer space of propellants and other materials.

## 4. Physics of Metals

G. Arai, M. Doyama, S. Eckstein, Y. Eckstein, L. Guttman, R. Huebener, J. Ketterson, H. Kierstead

The general objective of this program is to gain a more thorough understanding of metals and alloys especially with respect to their electronic structure, defect structure and radiation damage, their order-disorder and phase transformation properties, and their atomic diffusion processes.

### a. X-Ray Diffraction Studies

G. Arai and L. Guttman

Measurements of the x-ray diffuse scattering from a Fe<sub>3</sub>Al single crystal provide information about the state of order, that is, the spatial distribution of the two kinds of atoms present, in the neighborhood of the critical temperature. The Fe-Al system shows two phase transitions for the approximate composition of Fe<sub>3</sub>Al. The lower one is at 550°C; the upper one varies somewhat, about 790°C. These studies will be followed by investigations of other binary systems.

b. Fermi Surface Studies in Semi-Metals  
S. Eckstein, Y. Eckstein and J. Ketterson

Measurements of the magneto-resistance and ultrasonic-attenuation in bismuth, antimony, and arsenic have been made. Analysis of Shubnikov-de Haas measurements carried out to 25 kilogauss with antimony shows that there are two sets of carriers both having ellipsoidal character. Similar measurements with bismuth showed no evidence of a third or fourth carrier. Measurements were also made with arsenic but the work is complicated because of difficulties in obtaining a suitable single crystal. The capabilities of the ultrasonic and high magnetic field equipment will be extended and future work will involve studies of other materials.

c. Quenching Studies in Metals  
M. Doyama, R. Huebener and J. Jackson

The enthalpies of formation and migration of single lattice vacancies in platinum have been determined, and estimates have been made of the vacancy pair binding energy. Defects introduced in platinum are observed through the changes they cause in the electrical resistivity and yield stress. The kinetics of aggregation of vacancies into clusters is being inferred from hardness measurements and will be observed by electron microscopy.

Equipment is being assembled for studies of the properties of point defects in copper. The formation energy and the activation energy for motion of a vacancy in copper will be determined. The behavior of the annealing will also be investigated.

Thermoelectric measurements with quenched gold wires in the temperature range 4°K to 220°K have yielded the following results: (1) vacancies cause a reduction in thermoelectric power; (2) an appreciable change in the phonon drag part of the thermoelectric power due to vacancies is observed; and (3) the phonon scattering cross section of vacancies is one to two orders of magnitude higher than expected from the mass scattering mechanisms.

d. Low Energy Ion Bombardment  
H. Kierstead

A radio-frequency plasma low-energy ion bombardment source is being used to study the mechanism of displacing collisions at energies below 100 volts. A series of experiments is now in progress in cooperation with the graphite research group to determine the displacement threshold of graphite for ions incident along the hexagonal axis. Studies will also be made of the range of displaced atoms produced at the surface of thin evaporated gold films to better understand the very low energy processes involved in radiation damage.

## C. Interaction of Nuclear and Particle Radiations with Matter

### 1. Inelastic Scattering of Subthermal Neutrons

D. Connor and J. Rush

The spectroscopy of inelastically scattered slow neutrons is unique as a powerful technique for the study of atomic motions in matter. The cold neutron facility at Argonne, placed in operation in May, 1963, has produced useful research results on the nature of hindered rotations in ammonium halides, optical vibrations in ionic crystals, and lattice vibrations in amorphous solids. A systematic study of the coherent scattering from polycrystals has been started.

The present preliminary cold neutron facility employs beryllium-filtered neutrons and a single scattering angle ( $90^\circ$ ). Current equipment development work should lead to later major improvements in resolution (multi-chopper velocity selector), neutron economy (simultaneous detection at several angles) and intensity (cryogenic moderator).

New research programs planned include intensive study of molecular motions in liquids and the study of incoherently scattering (hydrogenous) molecular single crystals in order to elucidate the complicated scheme of lattice vibrations.

### 2. Radiation Damage to Various Solid Materials

W. Primak, W. Buck and Y. Dayal

The general goal of the program is a more thorough understanding of the influence of various solid state structures on sensitivity to damage. In current studies a variety of radiation sources available at Argonne are being used to explore and resolve different radiation effects. The experimental approach is that of comparing the behavior of induced properties of various substances as the radiation is altered in kind and energy.

Studies on silica recently completed or in progress include: damage and internal stress in specimens exposed in nuclear reactors, internal stress in particle bombarded silica, surface crazing, ionization-annealing of compacted silica.

The energy dependence of the radiation effect in silica and germanium is being studied. Lenticular cavities and exfoliation have been found in corundum, spinel, rutile, and peridot which had been bombarded with protons or helium ions in the 100 keV region.

The temporary enhancement of the electrical conductivity occurring when materials which normally are poor conductors are subjected to ionizing radiation is being studied using the linear accelerator. The current interest is centered on the solvated electron, or "polaron", and the "hydrated" electron.

#### D. Low Temperature Physics

O. V. Lounasmaa, H. Kierstead, J. Ketterson and Y. Eckstein

The low temperature physics program includes the studies of the properties of liquid helium itself and precision low temperature calorimetric studies of various materials designed to obtain nuclear, lattice and electron contributions to specific heats. The low temperature physics group also operates the Collins liquifier and furnishes liquid helium to other groups.

Precision measurements of the thermodynamic behavior of helium-4 very near the lambda-curve are in progress using temperature intervals of the order of  $10^{-5}$  degrees. Attempts to measure some properties of sound propagation in liquid helium-3 and helium-4 are underway in cooperation with B. Abraham of the Chemistry Division.

A helium-3 cryostat is being used for low temperature specific heat measurements. Investigations on a number of the rare earth metals in the temperature range  $0.4^{\circ}$  and  $4^{\circ}$ K have been very successful. Studies on other samples will be made. Measurements at still lower and at higher temperatures are anticipated in future program plans.

#### E. Solid State Theory

The solid state theory program has as its general objective the development and application of new theoretical techniques and concepts and the application of existing methods and concepts to give a better understanding of the nature of solids. The program is intended to give a theoretical interpretation of experimental results and also to give aid in the choice of the most important and fruitful experimental endeavors. The following projects are typical of the work:

##### a. Properties of Ionic Solids and Lattice Dynamics F. Fumi and M. Tosi

The determination of the cohesive energies and the apparent sizes of ions in the alkali halide crystals, based on the Born model semiempirical description of the interionic forces, has been completed. While the electrostatic interaction of point-like ions accounts for most of the cohesive energy of typical ionic crystals like the alkali halides, the description of the interionic forces involves also terms associated with the overlap of the electron clouds of the ions, which are of considerable interest in themselves and of paramount importance in determining other physical properties of these crystals.

General theoretical expressions for the temperature dependence of the thermodynamic functions of non-metallic crystals, and of the associated Debye temperatures, can be derived from statistical-mechanical principles. A fit of such expressions to accurate experimental data on the thermal thermodynamic functions (entropy, thermal energy, and heat capacity) for various types

of non-metallic crystals has been undertaken. An investigation of the thermodynamic properties of solid argon, leading to a determination of the first few moments of the vibrational frequency spectrum and of the anharmonic and defect contributions to the free energy, has been initiated.

b. Dynamics of Atomic Motions in Liquids and Solids

A. Rahman, K. Singwi, F. de Wette and J. Kokkedee

Clues to the understanding of atomic motions in liquids and solids are furnished by slow neutron scattering, light scattering, and dielectric dispersion. All three of these fields have been explored theoretically and the results compared with available experimental data. The scattering by water of slow neutrons has been studied extensively. These studies are of great fundamental importance but also of immediate practical importance to problems of neutron thermalization in reactors. A fast computer has been used to simulate atomic motions in liquid argon. These studies have been singularly successful and point to more extensive uses of computational facilities for further statistical studies of liquid behavior. Work on dielectric relaxation in polar liquids from the space-time correlation function approach is also in progress.

c. Electronic Properties of Solids

F. Bassani and J. Robinson

The general areas of primary interest continue to be the direct calculation of band structures both within the one-electron approximation and as extended to include electron correlation effects, and the calculation of and extraction of information from electronic transport properties. Calculations have been completed of the valence and conduction bands of several III-V compounds and IV elemental semiconductors and of AgCl. Conduction bands have been computed, in a point ion approximation, for several alkali halides.

In degenerate samples of some many-valley semiconductors the effectiveness of dielectric screening by the conduction electrons can be changed drastically and abruptly by small changes of donor concentration. A theoretical study of this effect, in cooperation with S. Rodriguez at Purdue, has led to a reasonably complete understanding of experimental results on doped germanium. The work suggests the strong change in screening should lead to measurable changes in a variety of other properties, including NQR and Knight shift and all oscillatory quantum effects in high magnetic fields.

d. Exchange Coupling and Magnetism

T. Arai

A technique similar to those in many-body problems has been developed which permits a rigorous calculation of the Heitler-London energy and exchange coupling to be carried out without

difficulty for insulators and semiconductors in which the spins and magnetic moments whose alignments lead to magnetic effects can be localized. That is, a concrete mathematical basis now exists for the localized model. In metals, the more difficult question exists as to whether d-electrons are itinerant or localized and what the mechanism of the exchange interaction is. To facilitate such discussion, it is proposed to construct a new method combining the Heitler-London method already developed with the orthogonalized plane wave approach.

e. Interaction of Sound and Conduction Electrons  
S. Eckstein

The propagation of sound in a material containing conduction electrons produces a direct current of the electrons, proportional to the intensity of the sound. Expressions have been found for the acoustoelectric current in a material containing either electrons alone, or containing both holes and electrons. The presence of external electric and/or magnetic fields was assumed. In some cases the acoustoelectric current opposes the usual direct current for amplification of sound conditions. In semi-metals, such as bismuth, the acoustoelectric current reinforces the usual direct current for amplifying conditions.

A more complete theory of geometric resonances in the magneto-acoustic attenuation of sound has been worked out and is proving useful in the mapping of Fermi surfaces. Further extensions of the theory are in progress.

f. Ab Initio Calculations on Atoms and Molecules  
P. Bagus and T. Gilbert

Analytic Hartree-Fock calculations for all terms of the ground configurations of He through  $\text{Na}^+$  have been completed, including a careful analysis and tabulation of the expansion error (a crucial point for subsequent use of these results). Other work includes the calculation of x-ray states of six selected atoms; a generalization and systematization of the formalism for obtaining Hartree-Fock equations for localized orbitals in crystals; LCAO calculations of the valence bands in certain alkali halides; and calculation of certain properties of self-trapped holes in these crystals. The calculations of x-ray states revealed the interesting and important result that the correlation between electron pairs depends strongly on the manner in which the shells are occupied, contrary to the assumption on which many current analyses of the correlation energy are based.

g. Correction Terms to the Hartree-Fock Equation  
Lars Hedin

The Hartree-Fock equation for many electron systems can be regarded as a first approximation to a more general equation where the energy eigenvalues are the exact excitation energies for the

system under consideration. The first correction term to the H-F equation, the Random Phase Approximation (RPA), has been discussed in considerable detail and evaluated numerically for an electron gas. The question of the accuracy of the RPA in the metallic density region has been treated and the corrections to a band-calculation for a real solid have been evaluated using the OPW-formalism.

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**Contract:** Associated Universities, Inc.  
Brookhaven National Laboratory

**Contract Number:** AT-30-2-GEN-16

**Present Contract Term:** June 30, 1967

**Cost to AEC:** \$654,000

**Contract Title:** BASIC RESEARCH IN THE METALLURGY DIVISION

**Investigators:** David H. Gurinsky, Head, Metallurgy Division,  
and staff

**Scope of Work:** A. Liquid Metals

J. R. Weeks, S. G. Epstein, A. Paskin

A better understanding of the mechanisms of the reactions between solid and liquid metals is being sought. This requires further knowledge of the structural and chemical properties, the migration of solute atoms through liquid alloys, and the energy of adsorption of liquid metals on solid metals. During FY 1964, electrodiffusion studies of Ag, Cr, and Fe in Bi have been completed. Solubilities of Fe, Co, Cr, Cb, Ta, Ti, Zr in Hg were obtained at temperatures up to 775°C. A stress-sensitive selective leaching of Zr from Cb-1Zr by Hg and Bi was discovered and studied. A relationship between solubility thermodynamics and liquid-solid interfacial energies was postulated which is potentially useful in predicting systems sensitive to liquid metal embrittlement; it was predicted (and experiment proved) embrittlement of Cb and Cb-1Zr in Bi as well as Hg. The small emf's of liquid metal free-energy cells can be correlated to thermodynamic activities and electrodiffusion mobilities.

Work on Bi and Hg was terminated in favor of a more basic study of liquid alloys. An experimental and theoretical program was initiated on a single systematic series of alloys with Na as a solvent and the remaining alkali metals plus Cu, Ag, Au, Cd, In, Sn, and Sb as solutes. Properties to be measured include thermodynamics, molar volumes, electrical resistivities and Hall constants at constant volume, thermoelectric power, viscosity, diffusivity, and electrodiffusivity. The alloys are selected to evaluate size, mass, and valence effects on these properties.

B. Fission Fragment Damage

J. J. Kelsch, A. Paskin, O. F. Kammerer

The mechanisms of fission fragment damage in thin films are being studied. Theoretical calculations have been made on a model which examines the physical conditions which enable track formation. Experiments are in progress to test the details of the model using U<sup>235</sup> as the fission fragment source.

The work is mainly concerned with: (1) creating metal films by evaporation and measuring their thickness, electrical conductivity and particle size (2) correlating the film continuity and other physical properties of the film with the ability to produce tracks (3) examining the role of the substrate in composite films (4) understanding the role of various layers in a composite film such as Pt-UO<sub>2</sub>-Pt (5) studying the ability of fission fragments to produce tracks in the initial and final portions of their range (6) understanding the different mechanisms of track formation in insulators and metals (7) developing theoretical models and making quantitative calculations on energy transfer mechanisms to account for the observations in metals and insulators.

### C. Superconductivity

D. G. Schweitzer, A. Paskin, O. Kammerer, M. Strongin

The program is concerned with studying superconducting materials. Efforts are directed at obtaining information on (1) the role of irradiation defects and metallurgical structure on superconducting properties (2) flux trapping and annealing in irradiated and unirradiated type II and type III superconductors (3) phonon spectra and the energy gap in superconducting materials joined by thin insulating films (4) Hall effects in the region between H<sub>c2</sub> and H<sub>c3</sub> (5) superconducting properties of stoichiometric and non-stoichiometric carbides and (6) superconducting behavior of composites of type II and type III materials.

Observations have been made of the surface superconductivity in types I and II superconductors. The ac susceptibility technique has also been used to study the temperature dependence of the Ginsburg-Landau parameter, which is particularly important in high-field superconductors.

### D. Thermodynamics of Refractory Carbides

S. Aronson

An investigation of the thermodynamic and electrical properties of refractory metal carbides, nitrides and borides is underway. Nonstoichiometric regions in these compounds are being studied in an effort to obtain a better understanding of the nature of the chemical bonding and electronic structure in these compounds.

The free energies, entropies, and enthalpies of formation of thorium monocarbide and thorium dicarbide have been obtained from measurements on solid electrochemical cells at 800-1000°C.

### E. Mechanical Properties of Body-Centered Cubic Metals

J. G. Y. Chow and S. B. McRickard

This program is concerned with studying the effect of neutron irradiation on the mechanical properties of body-centered cubic metals. Pure Fe and other metals with the bcc lattice structures are being presently studied. The effort is directed at obtaining information about: (1) mechanism of irradiation hardening, yielding and plastic deformation, embrittlement, fracture, and

increase in ductile-to-brittle transition temperature; and (2) the microstructure and dislocation substructure as revealed by the electron microscope.

#### F. Irradiation Damage in Graphite

D. G. Schweitzer, S. Aronson, R. M. Singer

The objectives of this program are to determine and understand the neutron-induced property changes in irradiated graphites. These studies include an investigation of the defects produced and their reactions upon further reirradiations and annealing. The studies involve analysis of dimensional, lattice, stored energy, thermal electrical, magnetic and oxidative changes in these types of graphites.

#### G. Mechanism of Gas Diffusion in Carbides

A. Auskern

The object of this program is to study diffusion mechanisms in carbides. The technique of rare gas diffusion is being used, employing xenon 133. The gas may be introduced into the solid by uranium fission recoil. Diffusion coefficients are a function of the subsequent rate of release of the xenon from the carbide.

In addition to the diffusion experiments, much effort is spent in preparing suitable materials, characterizing them, and investigating any properties which might have an effect on diffusion.

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Contractor: Brookhaven National Laboratory, Upton, L. I., New York

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Contract Title: BASIC RESEARCH IN THE SOLID STATE DIVISION

Investigators: G. J. Dienes and Staff

Scope of Work:

The basic aim of this solid state research program is the understanding of the interaction of neutrons, charged particles and ionizing radiations with solids. Such understanding is of fundamental as well as practical significance. The general program is conveniently divided into three complementary activities. A. Radiation effects, produced by reactor and  $\gamma$ -irradiations, are being studied by means of changes in many physical properties. While the main emphasis is on radiation effects, other departures from perfect periodicity are under active investigation. Metals, insulators and organic materials are being studied by a variety of techniques. B. Neutron diffraction and neutron inelastic scattering are being used for structural studies on metallic, magnetic and ferroelectric crystals. These studies are directed at fundamental questions in the theory of solids, theory of magnetism and the character of crystal transitions. C. Theoretical work, closely related to the overall program, is in progress on a variety of problems within the field of defects in solids, vibrational spectra of crystals and magnetism.

A. Radiation Effects

1. Optical and Resonance Studies of Insulators.  
P. W. Levy, P. Townsend, S. Kalbitzer.

The study of the effects of strain on color center formation and the effects of radiation on mechanical properties in the alkali halides is being continued. Recent results indicate that straining a NaCl crystal modifies the well known relation between the M-center and F-center concentrations. This relation is usually stated as follows: The M-center concentration  $\alpha_M$  is proportional to the square of the F-center concentration  $\alpha_F$ , or  $\alpha_M = (\text{const})_1 \alpha_F^2$ . A modified form of this equation  $\alpha_M = (\text{const})_1 \alpha_F^2 + (\text{const})_2$  applies to crystals that have been strained. It was found that the additional term,  $(\text{const})_2$ , increases with increasing strain. The exact dependence is yet to be determined. As an example of the effects of irradiation on mechanical properties, the changes in yield point of NaCl with increasing gamma-ray dose have been investigated. The yield stress, Y, of un-irradiated NaCl is about 10-30 Kg/cm<sup>2</sup>. It increases monotonically with increasing gamma-ray dose to about 200 Kg/cm<sup>2</sup> for irradiations of  $6 \times 10^7 R$ . There is a large

change in slope at about  $5 \times 10^6$  R which is apparently related to the defects present. This can be demonstrated by the behavior of M-centers. In crystals subjected to less than  $5 \times 10^6$  R, the M-center concentration, which is relatively low, decreases with time after the irradiation. In contrast, in crystals subjected to more than  $5 \times 10^6$  R the M-center concentration is about four times larger and increases after the irradiation is completed.

The gamma-ray irradiation facility, which provides a means of making optical absorption measurements on samples while they are being irradiated, is being used to study the growth and annealing of F-centers in KCl. The study of the formation of F-centers as a function of dose rate at room temperature has been completed. The initial coloring was found to be proportional to total dose, i.e., independent of dose rate. In this region approximately 100 eV must be deposited in the crystal by the gamma-ray field to produce one F-center. The initial portion is followed by a region in which a steadily increasing dependence on dose rate prevails. The stability of the KCl F-center at room temperature was determined by coloring the crystals to saturation and then "turning off" the gamma-ray field. The F-center concentration is then measured for periods of time which extend from a few seconds to several days. There is an initial rapid decay, which is roughly the same in all crystals, followed by a very slowly decreasing component. From isothermal annealing measurements the kinetics were found to be bimolecular suggesting that the F-centers are destroyed by the recombination of the electrons trapped on vacancies with the holes that have formed V-centers. This mechanism is supported by the observation that the V-centers are formed by irradiation and disappear as the F-centers disappear.

Detailed electron spin resonance studies are in progress on sodium bromate. Large crystals of this material have been grown. These are so pure that it has been impossible to detect any ESR signals in them prior to irradiation. When a pristine  $\text{NaBrO}_3$  sample is irradiated with ultraviolet light at room temperature, it becomes colored, but an ESR signal is not detected. If the sample is then irradiated with gamma rays, its color is increased but still no ESR signal is present. When the crystal is then subjected to additional ultraviolet light an ESR signal grows in until it reaches a saturation level and additional color is developed. Upon repetition of this process it is found that the saturation level ESR signal and the color center concentration are nearly proportional to the total gamma-ray dose.

## 2. Effect of Irradiation on Solid State Reactions

G. J. Dienes, A. C. Damask, R. A. Arndt

A study of the effect of neutron irradiation of Al-Cu, a precipitating alloy, is in progress. It was anticipated that the severe local damage associated with a displacement spike could serve as a nucleus for precipitation and that an acceleration of the precipitation process could be observed. (This effect has been observed and studied in Fe-C alloys at this laboratory). Preliminary experiments on a Al-Cu (1%) alloy have shown that neutron irradiation of about  $10^{16}$  nvt (fast) causes the resistivity decay curve at  $110^\circ\text{C}$ , associated with the late GP zone or early  $\theta'$  phase, to be accelerated by a factor of 2 to 3. The irradiations are performed at ambient temperature and the annealings are performed outside of the reactor following the irradiation. The results therefore indicate that the observed acceleration cannot be caused by enhanced diffusion and must be associated with some microscopic structural change in the alloy.

### 3. Effect of Irradiation on Diamond

D. T. Keating, R. Perret.

Measurements on the small angle scattering of x-rays from single crystals of irradiated diamond are in progress. These measurements using film techniques are being used to survey the effects of neutron exposure and crystal orientation on the small angle scattering. Small angle x-ray scattering measurements yield information on the nature of defects by giving a measure of the fluctuation in the density from the mean density as a function of correlation distance.

### 4. Effect of Irradiation on Organic Crystals

R. A. Arndt, A. C. Damask.

The basic techniques for the study of the electrical properties of organic crystals have been developed and the measuring apparatus assembled. It was recognized that the organic crystals had to be of very high purity to exhibit reproducible properties. Precipitation procedures by chromatographic columns, vacuum sublimation, and zone refining were established, as well as crystal growing techniques to produce single crystals of desired orientation. Anthracene crystals containing less than 10 ppm of impurities have been grown.

## B. Neutron Diffraction

### 1. Magnetic Structures

R. Nathans, G. Shirane, H. Alperin, S. J. Pickart.

Detailed measurements are being made on a natural single crystal of fazalite,  $\text{Fe}_2\text{SiO}_4$ , since powder data gave evidence of a non-collinear antiferromagnetic spin arrangement. The temperature dependence of the intensities of magnetic reflections shows that one component of the antiferromagnetic arrangement appears around  $60^\circ\text{K}$ , followed by the other at  $30\text{-}40^\circ\text{K}$ . Non-collinear magnetic structures have also been found over a wide composition range between ferromagnetic CrTe or MnSb and antiferromagnetic CrSb. Detailed measurements as a function of temperature have been made on selected compositions in order to determine the direction and magnitude of the various spin components.

Several spiral type oxides containing predominantly  $\text{Cr}^{3+}$  on octahedral sites have been studied.  $\text{FeCr}_2\text{O}_4$  has a cone spiral type of spin structure, in agreement with theoretical predictions and indicating relatively strong negative exchange interactions between the Cr ions.  $\text{FeCr}_2\text{S}_4$ , however, is a simple Neel type of ferrimagnet.

The spin structures of the binary fluorides with chemical formula  $\text{XMnF}_3$  ( $X = \text{Na}, \text{Rb}, \text{Cs}, \text{and } \text{NH}_4$ ) have been investigated by means of powder neutron diffraction measurements at low temperatures. Considering only the lattice of  $\text{Mn}^{2+}$  ions and neglecting the departures from cubic symmetry, we find the antiferromagnetic lattice of the compounds with  $X = \text{Na}, \text{Rb}, \text{and } \text{NH}_4$  to be of the same basic type. It consists of a doubling of the unit cell in three directions, so that each Mn spin is surrounded by six antiparallel nearest neighbors, as was found previously for  $\text{KMnF}_3$ .  $\text{CsMnF}_3$ , however, is related to the hexagonal modification of  $\text{BaTiO}_3$  in which the hexagonal stacking sequence is altered. The antiferromagnetic ordering is confirmed by neutron diffraction.

A diffraction study of a single crystal of gadolinium has removed an ambiguity in the magnetic structure of this metal. A single crystal disc of Gd cut parallel

to (00.1) has been studied in zero magnetic field. A careful search along and perpendicular to the c-axis in the neighborhood of the (00.2) reflection has failed to reveal any satellites in the temperature range 77°K to 290°K. Thus, unlike the rare earth elements from Tb to Tm, gadolinium is a normal ferromagnet. Above 248°K the moment is aligned along the c-axis. Below this temperature, the moments make an angle with the c-axis which reaches a maximum of 75° at 195°K and approaches 30° at 4°K.

## 2. Spin Density Distributions

G. Shirane, R. Nathans, H. Alperin, S. J. Pickart.

The unpaired electron density in the intermetallic compound ZrZn<sub>2</sub>, reported to be ferromagnetic by Matthias and Bozorth, has been investigated. The magnetic scattering is very small but is readily observable with the highly sensitive polarized beam technique. The results show that the moment is almost entirely on the Zr atoms and is more diffuse than one would expect for a 4d electron distribution, suggesting possible polarization of the 5s conduction band. Moreover, there is definite evidence for movement of electrons into the tetrahedral bonds joining Zr atoms; the considerable spin density along these bonds indicates that a localized model is inappropriate for explaining the ferromagnetism.

The distribution of magnetic moments in the Fe-Rh system has been investigated by neutron diffraction in the composition range between 35 and 50 atomic % Rh. These alloys have chemical order of CsCl type; the body corner positions are occupied by FeI atoms and the body centers by Rh and FeII. The magnetic moments in ferromagnetic alloys containing 35, 40 and 48% Rh are  $\mu_{\text{FeI}} = 3.1 \mu_B$ ,  $\mu_{\text{FeII}} = 2.5 \mu_B$  and  $\mu_{\text{Rh}} = 1.0 \mu_B$  at 25° C. The moment of the FeI atom in the 50% Rh alloy, which is antiferromagnetic at room temperature, increases to 3.3  $\mu_B$ . A detailed study of the unpaired spin density distribution in the 48% Rh alloy was made by the polarized beam technique. While the FeI atom has a nearly spherical density distribution, that of the Rh atom shows a strong tendency towards  $e_g$  symmetry.

## 3. Non-magnetic Structures

B. C. Frazer, A. Goland, B. Mozer, G. Will, R. Segnan, D. Cox.

A number of crystals having the tetragonal scheelite structure have been examined by X-rays. These studies have yielded the heavy atom positions, but in most cases the oxygens could be located only from packing considerations, and in all cases the uncertainty in the oxygen position is quite large. With neutron diffraction data direct refinement of all parameters is possible. Starting with the oxygen coordinate parameters of Sillén and Nylander, a preliminary set of single crystal (h0l) neutron data was refined by least squares to yield  $x = 0.2417 \pm 0.0007$ ,  $y = 0.1522 \pm 0.0009$ ,  $z = 0.0861 \pm 0.0002$ . These may be compared to the set proposed by Sillén and Nylander:  $x = 0.25 \pm 0.02$ ,  $y = 0.15 \pm 0.02$ ,  $z = 0.075 \pm 0.015$ . An appreciable change is noted in the z parameter although the neutron value falls within the rather large estimated error limits. While the new results appear to be quite reliable, some further study will be carried out to investigate possible extinction effects using the original  $c$  axis crystal and another crystal in a [110] orientation.

Scattering of cold neutrons by light water and salt solutions is under investigation by means of the filter-cutoff technique. The method has been refined in order to make optimum use of the low flux of cold neutrons provided by the Brookhaven Graphite Reactor, and to remove certain experimental uncertainties encountered by

others using the same technique. Energy resolutions of 2.5 percent and one percent have been achieved. Broadening of the quasielastic peak has been observed as a function of scattering angle, but no evidence of low-energy quantum transitions has been found. Measurements on a concentrated solution of NaCl do not show a decrease in the broadening although it is known that the coefficient of self-diffusion of H<sub>2</sub>O in this solution is about 25 percent less than the pure water value. The data are being compared with various theories of cold-neutron scattering by liquids.

Room temperature Mössbauer spectra have been obtained for Fe<sup>57</sup> in the following h.c.p. metals: Cd, Co, Dy, Gd, Mg, Ru, (Se), (Te), Ti, Zn. Co<sup>57</sup> was diffused into these metals and used as the source. The absorber was 3.85 mg/cm<sup>2</sup> of ferrous potassium cyanide. The isomer shift and the quadrupole splitting give information about the charge density and electric field gradient of the conduction electrons at the iron nucleus. The field gradients determined from the experiment show a c/a dependence in qualitative agreement with De Wette's calculation for a point ion model and a uniform conduction electron density. The isomer shifts obtained from the measurements are not fully explained by using conduction electron densities of the pure host metals. The measured isomer shifts could be explained if the iron impurity is considered to be charged and screened by the conduction electrons of the host metal. The screening charge would also contribute to the field gradient at the Fe<sup>57</sup> nucleus and might account for the differences in the observed field gradients and De Wette's results.

Cold neutron inelastic scattering experiments have been performed on niobium and molybdenum. Estimates of the vibrational frequency distribution have been obtained from these experimental data.

Considerable effort has been directed towards the organization of the materials laboratory, particularly with respect to providing facilities necessary for the growth of a wide variety of single crystals of suitable size for neutron diffraction investigations. Facilities now include an arc-melting furnace, Bridgman and Czochralski (crystal pulling) equipment, various other high temperature furnaces, a hydrothermal unit and an electron beam zone melting furnace. A Spark erosion machine for strain-free cutting and shaping of metal samples, and a controlled atmosphere "dry-box" for handling sensitive materials have been acquired recently.

### C. Theory

#### 1. The Dynamics of Radiation Damage C. Erginsoy, G. H. Vineyard

Studies on the dynamics of radiation damage in b.c.c. lattice ( $\alpha$ -iron) have been continued and extended to higher knock-on energies. The probability of di-vacancy production by a 100 eV knock-on was calculated by running over fifty dynamic events in a large variety of initial directions to simulate isotropic distribution. At higher energies the effects of lattice anisotropy on the number of defects created was studied. A sequence of non-productive replacement sequences is caused by a knock-on in a penetrating direction, i.e., between the low-index crystal directions.

Recent experiments show that a small fraction of a beam of heavy ions incident on a clean single crystal surface penetrates deeply (several microns) into the crystal lattice. Such collisions provide a new means of studying the non-adiabaticity of slow atomic collisions involving large angular momenta. Unique conditions exist in channels because (a) impact parameters are independent of ion energy and are precisely

known, (b) the same atom makes a rapid succession of collisions with essentially constant impact parameter and kinetic energy. Calculations show that rare gas atoms can be multiply excited in their outer shells and lose electrons by auto-ionization in such collisions. A consequence of this process is enhanced penetration into the crystal lattice because the interaction potential governing their slowing down will be greatly reduced after ionization. A model based on such collisional excitation and auto-ionization of channeled atoms explains the observed experimental results satisfactorily.

## 2. Point Defects and Interstitial Atoms in Iron

R. A. Johnson, A. C. Damask, G. J. Dienes.

Calculations concerning the nature of point defects have been carried out with a lattice model simulating  $\alpha$ -iron using high speed computer techniques. Iron interstitials, carbon interstitials, lattice vacancies, and various small clusters of these have been studied. The atomic configuration, the motion energy, and the motion volume have been determined for the different defects, and agreement with experiment, where available, is good. The iron interstitial migration energy was found to be 0.3 eV, which indicates that Stage I radiation damage annealing in  $\alpha$ -iron proceeds by free interstitial migration. The carbon interstitial calculations tend to confirm and augment the model proposed to explain experimental results on the iron-carbon system. The iron-carbon interaction was represented by a cubic equation with the parameters chosen to yield the experimental value for the carbon migration energy and activation volume, and the binding energy of a carbon atom to a vacancy. With this model the approximate experimental value of the energy of a carbon atom in solution in iron relative to  $\text{Fe}_3\text{C}$  was obtained. When the constants of this form of the iron-carbon potential are scaled to nitrogen in iron and nitrogen in vanadium, the experimental activation volumes for diffusion of nitrogen, effectively zero in iron and 0.14 atomic volumes in vanadium, are obtained.

## 3. Defects in Alkali Halides

G. J. Dienes, R. D. Hatcher.

The distortion around and the relaxation energy for a  $\text{Cl}^\circ$  interstitial atom in a NaCl lattice has been obtained for various positions of the  $\text{Cl}^\circ$  by a method involving the exact calculation of electrostatic, polarization, dipole-dipole and repulsive energies. The relaxation of the order of twenty neighboring ions has been taken into account. The following positions of the  $\text{Cl}^\circ$  were investigated: the cube center, the face center and various positions along the cube and face diagonals. The cube center and cube diagonal positions were always found to be stable relative to the face center and face diagonal positions. There are two energy minima of almost the same value along the body diagonal, one in the center of the cube and one straddling a  $\text{Cl}^\circ$  lattice position. These two minima are separated by a potential barrier of about 0.2 eV. The energy differences for the various configurations along the face diagonal are small with the face center the position of lowest energy. The face center position is metastable with respect to the body centered position by about .03 eV. The energy difference between the body centered and face centered positions is 0.44 eV, giving an activation energy along this line of motion of 0.47 eV.

## 4. Theory of Fission Track Formation

A. Goland, A. Paskin.

A model has been proposed to explain fission-fragment tracks in thin polycrystalline metal films. The model predicts that the fragment energy will be trans-

ferred to the electrons within a crystallite, and thence to the lattice, causing evaporation provided certain conditions are satisfied. One is that the energy per atom imparted to the lattice by the electrons exceeds the sublimation energy. Another, is that the competing process of thermionic emission from the crystallite is quenched because the crystallite becomes charged. The latter condition implies that tracks will be observed in thin films of high resistivity, but not in those whose resistivity is about equal to the bulk value.

#### 5. Theory of Magnetism

M. Blume, A. Honma

The theory of polarized neutron scattering was extended to include spin-orbit scattering of neutrons. This was motivated by a recent experiment in which interference between spin-orbit and nuclear scattering was observed. The theory shows that in magnetic substances an additional effect due to interference between spin-orbit and magnetic scattering should be observable in a number of substances. This will provide a means for the measurement of the spin-orbit scattering amplitude. The theory of spin-orbit coupling in atoms was developed for rare-earth and 4d shell atoms and ions. Calculations of coupling constants from first principles showed good agreement with experiment. The spin-orbit coupling constants were related to hyperfine structure constants.

The spin-spin interaction in paramagnetic ions has been analyzed in detail. Calculations show that this interaction is of lesser magnitude than had previously been believed. A table of the spin-spin interaction constant for iron-series ion has been prepared. The theory of polarized neutron scattering by targets in which both the electrons and nuclei are polarized has been completed and has been used in the analysis of a transmission experiment on Holmium.

#### 6. Density of States

B. Mozer

X-ray emission spectra of metals have been used to deduce properties of the density of electron states below the Fermi energy. The density of electron states as deduced from X-ray emission spectra is expected to be different from the density of electron states of the metal in the ground state. This difference is caused by the hole in the valence band which perturbs the conduction electron density, especially in the vicinity of the hole. An approximate calculation of the perturbed density of states has been carried out by considering the hole in the valence band as an extremely localized impurity in the metal. The weighted density of electronic states associated with this impurity was derived in terms of a Green's function for the pure metal expressed in the Wannier function representation. The method has been used to obtain the perturbed density of states of Lithium using the density of states calculated by Ham for the pure metal.

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D. T. Keating, "Interpretation of the Scattering from a Liquid-like Binary," J. Appl. Phys. 34 (1963) p. 923.

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Contractor: Hanford Atomic Products Operation, General Electric Company, Richland, Washington

Contract Number: AT(45-1)-1350

Present Contract Term: July 1, 1963 through June 30, 1964 (Fiscal year 1964)

Cost to AEC: \$150,000

Contract Title: PLUTONIUM PHYSICAL METALLURGY RESEARCH

Investigators: T. K. Bierlein, R. D. Nelson, F. E. Bowman, H. E. Kissinger, and B. Mastel

Scope of Work:

This program is aimed at obtaining fundamental information on the physical metallurgical properties of plutonium, unalloyed and alloyed. Plutonium phases afford an opportunity for investigating monoclinic structures and the relationship between these structures and to various metallurgical properties.

The major effort is directed in two interrelated areas of investigation: (1) phase transformation and associated phenomena, and (2) processes and effects of deformation in monoclinic plutonium. A secondary effort is devoted to the development and application of a variety of supplemental techniques necessary for solving the relatively unique problems associated with the study of plutonium: optical and electron microscopy, X-ray diffraction, fractography, mechanical deformation, and precision density measurements. Electrorefined plutonium and as-reduced and vacuum-cast plutonium constitute the major source of the pure metal under investigation.

The time and temperature dependence of the various phase transformation kinetics have been established, and factors affecting the extent of physical damage during phase transformation and thermal cycling have been determined. Textured alpha plutonium will be employed in an investigation on the anisotropy of various physical properties of plutonium. Additional information on the mechanism of transformation of plutonium will be derived from changes in texture due to transformation. Studies of deformation and recovery processes, including stress relief, recrystallization and grain growth, will be pursued. The activation energies for normal creep in the plutonium

allotropes have been evaluated and experimentation will continue in the area of transformation creep. The effect of controlled additions of alloying constituents up to 0.1 atomic percent on the terminal kinetics of the beta → alpha transformation, which proceeds athermally, will be explored.

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F. E. Bowman and V. C. Asmund, "The Rolling of Alpha Plutonium," HW-80464, January 1964.

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R. D. Nelson, F. E. Bowman, and T. K. Bierlein, "Physical Damage of Plutonium," HW-80808, February 1964.

R. D. Nelson, F. E. Bowman, and T. K. Bierlein, "Steady State Creep of Plutonium," HW-80952, February 1964.

Contractor: Hanford Atomic Products Operation, General Electric Company, Richland, Washington

Contract Number: AT(45-1)-1350

Present Contract Term: July 1, 1963 through June 30, 1964 (Fiscal year 1964)

Cost to AEC: \$138,000

Contract Title: RADIATION EFFECTS ON METALS

Investigators: T. K. Bierlein, H. E. Kissinger, J. J. Laidler, and B. Mastel

Scope of Work:

The purpose of this program is to establish how neutron bombardment damages metals, how changes in the damage state occur during subsequent annealing treatments, and how impurity content influences the damage and recovery processes. Molybdenum, 99.99 percent pure, containing various amounts of carbon, nickel ranging from 99.4 to 99.997 percent purity with various substitutional impurities, and rhenium, 99.99 percent pure, to which tungsten or molybdenum will be added for decreasing stacking fault energy, are under study.

Program activities involve single crystal and polycrystalline specimens of these three metals, examples of different crystal systems. Information about the nature and degree of radiation damage and the postirradiation annealing mechanisms is obtained by correlating the results from various experimental techniques, such as transmission electron microscopy, X-ray analysis, mechanical testing, and stored energy release and electrical resistivity measurements.

The major portion of the experimental work to date has been performed on molybdenum. Transmission electron microscopy has revealed spot defects and loops in irradiated polycrystalline and single crystal specimens. The concentration of the defects as a function of irradiation dose and carbon content and their disappearance as a function of thermal treatments are being studied. Carbon appears to act as a nucleating agent for the defects

during irradiation up to  $10^{19}$  nvt. Accurate lattice parameter and length change measurements are supplying additional information on the nature of the defects present in irradiated molybdenum. After small amounts of deformation, the irradiated molybdenum develops "channels" within the defect structure. The mechanism of formation of these channels is currently being investigated. Explanations for the easy glide region and coarse slip lines observed in irradiated molybdenum single crystals are being advanced.

The combined effect of impurities and excess vacancies on the yield strength of nickel is being investigated as a precursor to irradiation experiments. The tendency for clustering of quenched-in vacancies is greater the higher the purity of the nickel; the hardening attributed to clustering of vacancies is reduced by the presence of impurity atoms. Mechanical property tests on quenched and aged specimens are being augmented by transmission electron microscope studies.

Future activities in the program will include studies of thermally activated deformation in irradiated molybdenum and nickel by strain-rate cycling techniques. These two metals, as well as rhenium, will be irradiated at controlled, elevated temperatures, and tests analogous to those being performed on specimens irradiated at 60 C will be conducted.

#### Recent Publications:

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**Contractor:** California, University of, Lawrence Radiation Laboratory

**Contract Number:** W-7405-eng 48

**Present Contract Term:** July 1, 1963 through June 30, 1964 (Fiscal Year 1964)

**Cost to AEC:** \$1,138,000.00

**Contract Title:** Basic Research on Metallurgy and Materials in the Inorganic Materials Research Division of the Lawrence Radiation Laboratory.

**Investigators:** L. Brewer, A. Searcy, and Associates

**Scope of Work:** The various program areas described below represent the current interests of the principal investigators associated with the Inorganic Materials Research Division. Almost all of the principal investigators are University staff members. More than two-thirds of the research staff are graduate students and temporary post-doctoral investigators. The overall program of the Inorganic Materials Research Division, including a Chemistry program of comparable size to that in metallurgy and materials listed here, is coordinated to meet two objectives: to provide a fertile interdisciplinary atmosphere for basic research accomplishment, and to prepare and train new talent in broad areas of fundamental research.

#### A. Properties of Metals and Alloys

##### 1. Kinetics of Dislocation Mechanisms

John E. Dorn

The major objective of this research program in mechanical behavior is the determination of the various dislocation mechanisms responsible for the plastic behavior of crystalline materials. This study requires consideration and development of suitable theories of dislocation mechanics, critical investigations of mechanical behavior of crystalline materials (particularly the determination of activation energies and volumes for deformation) compiled with auxiliary X-ray, metallographic and electron microscope evidence so directed as to provide documentation, and identification of the strain rate controlling deformation mechanisms. Specific areas of current interest include:

1. Mechanisms of low temperature prismatic slip in alpha solid solutions of Li in Mg.
2. On the low-temperature deformation of polycrystalline aluminum.
3. High-temperature creep of iron and iron alloys.
4. Recovery of creep induced substructures.

5. Effect of crystal orientation on strain hardening of aluminum.
6. The mechanism of deformation of AgMg at elevated temperatures.
7. Dynamic behavior of crystalline materials and plastic wave theory.
8. The rate-controlling mechanism of slip in the intermetallic compound Ag-Mg at low temperatures.
9. Mechanism for thermally activated slip in Ag<sub>2</sub>Al.
10. On the role of dislocations in the recovery of cold-worked aluminum.
11. Theory of dislocation constriction processes.
12. Impact of dislocation theory on engineering.
13. Nucleation of kink pairs and the Peierls mechanism of plastic deformation.
14. Recovery of creep resistance substructures.

2. The Fundamental Principles of High Strength Materials  
Earl R. Parker

In general, high strength materials tend to be brittle. From theoretical considerations, however, it has been concluded that high strength and ductility are not incompatible. Dislocation theory, in conjunction with alloy theory and control of process variables, can lead to an understanding of factors that control ductility in high strength alloy systems. The following areas of experimental research are intended to elucidate flow and fracture processes in complex multi-phase alloy systems:

1) Nitrogen Martensite: Zone refined single crystals of austenite with known orientations are being nitrided and subsequently transformed to produce a few large plates of nitrogen-martensite. The control of composition and orientation of both the austenite and the martensite in bulk and thin films permits a relatively unambiguous and detailed study of the structural features of martensite.

2) Theory of the Strength of Martensite: The currently accepted location of the interstitial carbon atom in martensite is between two iron atoms on the long edge of the unit cell. The space available at this position is considerably smaller than that of the adjacent site. A theoretical analysis has been made which shows conclusively that not only is the carbon in the more suitable tetrahedral site, but that carbon atoms form pairs in contiguous tetrahedral sites. Using the concept of carbon pairs, precise agreement of calculated and experimental lattice parameters has been obtained. Also, the model accurately predicts the crystal structure and lattice parameters of metastable epsilon carbide.

3) Internal Oxidation of Silver Alloys: Preliminary work on Ag-1 at % Mg-0 using transmission electron microscopy revealed no discrete particles in the system, even though hardening on oxidation is substantial. However, individual particles can be seen in internally oxidized Ag-1 at % Cd alloy. These two systems have been chosen for the study of dislocation-obstacle interaction. Cottrell-Stokes type of experiments are being carried out to study dislocation-obstacle dynamics.

### 3. Relation of Substructure to Properties of Crystalline Materials: Electron Microscopy.

Gareth Thomas

The relation of substructure and in particular lattice defects (dislocations, stacking faults, vacancies, solute atoms) to properties can be conveniently studied by employing the powerful technique of transmission electron microscopy which enables details of the order of  $5 \text{ \AA}$  or greater to be resolved. The general areas of research are as follows:

- 1) Body-Centered Cubic Materials: The effect of interstitial impurities upon dislocation arrangements of bcc metals and solid solutions and their effect upon mechanical properties.
- 2) Stacking Fault Energy: The stacking fault energy of fcc solid solutions is a function of composition and solute atom distribution. Estimates of SFE can be made from node measurements on electron micrographs. At present the following factors in relation to SFE are under investigation: (a) short range order; (b) mechanical twinning in shock loaded metals; (c) temperature.
- 3) Impurity-Vacancy Interactions: The concentration of quenched-in vacancies is a function of solute atom kind and concentration. The important parameter is the binding energy between vacancies and solute atoms. Estimates of this parameter can be made from dynamic measurements of dislocation climb rates using hot stage microscopy. The data will also be useful in understanding phenomena such as recovery and creep.
- 4) Defects in Silicon: This work is being done to understand the types and origin of lattice defects in undoped and doped epitaxial silicon.

### 4. Dislocation Studies

Jack Washburn

#### a. Dislocation Motion in Crystals Containing Vacancy Clusters

When dislocations move during plastic deformation, clusters of vacancies are left behind as part of the damage that causes strain hardening. Similar defects are also the cause of radiation hardening and are produced by quenching a crystal from elevated temperature so as to trap thermal vacancies. However, moving dislocations can also destroy some of these defects.

Therefore an understanding of the detailed interactions between moving dislocation and vacancy clusters of all sizes, from a divacancy up to voids or dislocation loops consisting of  $< 10^3$  individual vacancies, is fundamental to any real understanding of yielding and slip band growth in crystals.

Research in this general field during the year 1964 will be concentrated on the following measurements: (1) A study of the growth of vacancy clusters or small voids in quenched copper during low temperature aging. Small angle x-ray scattering techniques will be used. (2) Quantitative measurement of dislocation mobility in copper crystals containing vacancy clusters of known size.

#### b. Theory of Strain Hardening

Quantitative theories of strain hardening, the most successful of which has been that due to Seeger, have concentrated on an explanation of the second stage linear hardening of face-centered-cubic crystals; in particular those that have

been carefully annealed so as to produce initially a small density of dislocations. So far it has not been possible to propose more general theories because of the complexity of the changes in defect substructure that take place during plastic deformation. The shape of a stress-strain curve depends on so many variables that in spite of the vast amount of work in this field there are important aspects of the problem that have not been quantitatively studied.

Our research in this area during 1964 will consist of the following specific investigations.

1) The effect of initial dislocation substructure on yielding, on the hardening rate during stage I and on the transition to stage II will be studied using pure copper single crystals.

2) Experiments utilizing surface observations of slip bands will be conducted in an attempt to find out whether or not changes in the shape of stress-strain curves can be correlated with changes in the distribution of strain.

#### 5. Growth of Deformation Twins

Jack Washburn

Although the formal crystallography of twinning is well established, the mechanism of deformation twinning when considered on an atomic scale is far from being understood. In this respect our knowledge of twinning lags far behind our knowledge of deformation by slip.

Experiments are at present in progress to study the thickening of twin lamellae in zinc specimens deformed in tension. Normally this process cannot be studied closely because it occurs immediately after nucleation, under a rapidly decreasing load, and is accompanied by the nucleation of other twins. A technique has been developed for producing properly oriented cylindrical zinc tensile specimens the gauge section of which is traversed by a single twin lamella.

On deforming such a specimen at 20°C with the tensile axis in the basal plane the only process observed is the thickening of the twin lamella. This occurs by the smooth propagation of the two parent-twin interfaces at a constant load.

It is hoped to study the effect of shear stress and temperature on the rate of twin boundary propagation and to investigate the effect of grown in or introduced dislocation structures on the mobility of these boundaries. Present experiments are using specimens of 99.999% pure zinc.

#### 6. The Design of High Strength Materials From Fundamental Principles

Victor F. Zackay

The requirements for tough, ductile, high strength solids can be deduced from dislocation theory. By combining a knowledge of the thermodynamics and kinetics of phase transformations in metals with the precise control of process variables such as temperature, composition, and deformation, "ideal" microstructures can be approximated and the associated properties compared with those predicted from theory.

The following programs comprise the effort currently being devoted to the study of complex high strength solids.

1) Elevated Temperature Strain Aging: Highly alloyed martensitic steels are being strained varying amounts at different strain rates and temperatures. The volume fraction of finely dispersed carbides is significantly increased by this kind of processing.

2) The Spinodal Transformation: A characteristic of the spinodal transformation is the formation of composition gradients in a single phase solid. By appropriate choice of alloy systems, a ternary element can be diffused into the binary spinodal alloy. Compounds formed by this process are in a three-dimensional grid and the array can be closely controlled. The interaction of dislocations with grids of hard particles is being studied in both bulk and foil specimens.

3) The Liquid-Solid Transformation: The liquid-solid phase transformation can also be employed to produce controlled arrays of hard particles in ductile solids. One such system is that of aluminum and silicon with phosphorus added as an inoculant.

4) The Theoretical Strength of Solids: A comparison of the theoretical and actual strength-weight ratios of the common structural metals over a wide range of temperature has been made. The discrepancy between the theoretical and the actual strength-weight ratios at room temperature were shown to vary by factors ranging from approximately 3 for Fe and Ti, to about 40 for Be.

5) The Strain Hardening of Iridium: The metal, iridium, has a high elastic modulus ( $74 \times 10^6$  psi), is chemically inert, oxidation resistant to about  $1000^\circ\text{C}$ , and is reported to have an exceptionally high rate of work-hardening.

## B. Properties of Ceramics

### 1. Physical Ceramic Research

Richard M. Fulrath

This project is concerned with a study of the properties of polycrystalline and multiphase ceramic materials. A major effort is directed toward characterization of the microstructure of ceramic materials and understanding how a specific microstructure is formed. The mechanical properties and diffusional characteristics of polycrystalline and multiphase ceramics are strongly dependent on the microstructure and are of primary concern.

Specific areas of interest include:

1) Studies of composite systems with emphasis on alumina spherical particles dispersed in a glass matrix. The effort will concentrate on establishing the effect of the particle size of the dispersed phase on the mechanical properties of the composite.

2) Studies of the final densification in hot pressing  $\text{CaF}_2$ . The pretreatment of the alumina powders has given an indication of having a marked effect on the rate of densification and on the final density achieved and will be studied in detail.

3) The study of the permeation of gas through ceramics under stress, with emphasis on increasing the temperature at which the permeation is determined.

4) Studies will be initiated on the electrical and mechanical property changes induced in poling ferroelectric ceramics. The poling of a ferroelectric can induce considerable strain at grain boundaries in a polycrystalline body. These strains are believed to be responsible for loss of dielectric strength and failure of these materials when exposed to large electrical fields.

2. High Temperature Reactions, and Microstructure and Physical Properties  
Joseph A. Pask

The objective of this program is to gain a fundamental understanding of the factors responsible for microstructure of ceramic materials, and of the relationship of such microstructures to mechanical behavior at high temperatures. The research program may be divided into two principal areas: One is concerned with studies of the kinetics and mechanisms of reactions involving at least one nonmetallic inorganic solid phase; the second area is concerned with studies of the mechanisms responsible for the nature of the mechanical behavior of single crystals and subsequently the application of such knowledge toward a similar understanding of polycrystalline ceramic materials.

Specific areas of interest include:

1) Studies of the diffusion of iron into single-crystal MgO at temperatures up to 1600°C.

2) Studies of the diffusion of iron into sodium disilicate glass. Experiments will also be extended to include iron oxide-sodium disilicate glass diffusion couples.

3) Studies of the kinetics and mechanism of the dehydration of aluminum hydroxide.

4) The stress-strain behavior of polycrystalline MgO is being studied in relation to its microstructure including such variables as pore size and distribution, nature and amount of impurity, and nature of grain boundaries. The deformed specimens are being examined to determine the relative effects of dislocation movements and grain boundary sliding.

5) Plastic deformation studies of single-crystal specimens of a number of compounds with NaCl-type structures.

C. Thermodynamic Studies

1. Thermodynamics of the Metallic State  
Ralph Hultgren

1) The relative partial molar heat contents of Au and Sn in a liquid Au-Sn alloy will be measured in the liquid metal solution calorimeter. The change with composition of  $\Delta \bar{H}_{Au}$  and  $\Delta \bar{H}_{Sn}$  in the equiatomic region will be studied at a temperature just slightly above that of the melting point of solid AuSn, 691°K.

2) Heat capacity measurements on liquid alloys will be continued to determine whether the rapid decrease in  $C_p$  above the melting temperature found previously for Bi-In and In-Sn alloys is shown by other representative systems.

3) High-temperature heat contents ( $H_T - H_{298}$ ) and heats of fusion of the solid phases AlSb and InAs will be determined. Heat contents of liquid In-Sb alloys will be determined and combined with phase-equilibrium data in order to determine the partial molar enthalpies and free energies for the liquid alloys. Electrical-conductivity studies of In-Sb alloys presently in progress will be continued.

4) Galvanic cell studies will be made at elevated temperatures using a solid oxide,  $\text{ThO}_2$  (containing 8%  $\text{Y}_2\text{O}_3$ ), as the electrolyte. It is planned to determine the standard free energy of formation of some oxides, to measure the oxygen activity in dilute metallic solid solutions, and to determine the activity of the oxygen-saturated metal in some binary alloys. Systems with oxygen activities as low as  $10^{-34}$  can be investigated at temperatures up to  $1600^\circ\text{K}$ . The refractory metal-oxide systems selected for study are those of Ti, Zr, V, Nb, and Ta.

5) The heats of formation of the ordered and disordered phases of CuPt and thus the heat of ordering will be determined by liquid tin solution calorimetry.

6) The compilation and evaluation of published thermodynamic data for metals and alloys and possibly a few nonmetallic systems will be continued.

## 2. High Temperature Reactions, Mass Spectrometry

Alan W. Searcy

1) As part of a general effort to investigate the evaporation coefficient of alkaline earth dihalides, torsion furnaces will be used for measurements of equilibrium pressures of  $\text{SrF}_2$  by the torsion-effusion method, and for measurements of the free surface apparent pressure of  $\text{SrF}_2$  and  $\text{BaF}_2$  by the torsion-Langmuir method.

2) Nitrides studied to date, GaN, AlN, and  $\text{Be}_3\text{N}_2$ , have high free energies of activation for vaporization. Measurements of the vapor pressure and free surface sublimation kinetics for  $\text{Mg}_3\text{N}_2$  as functions of temperature will be initiated. Attempts will be made to correlate surface structure, porosity, and impurity level with variations in sublimation kinetics in order to obtain not only a free energy of activation for the vaporization process but also more detailed understanding of the factors that influence rates of evaporation.

3) A technique of determining the multiplicities of ground and low-lying electronic states with the inhomogeneous field magnet attached to the mass spectrometer will be tested and perfected on known species such as oxygen. The technique, if successful, will then be applied to the problem of establishing the ground electronic states for vapor molecules.

4) The theory of purification of metals by removal of carbon by use of controlled oxygen pressures will be explored for a variety of metals. A new method which would remove carbon and nitrogen simultaneously as HCN will also be theoretically evaluated.

5) The reaction of chlorine gas with tungsten will be studied at chlorine pressures of  $10^{-6}$  to  $10^{-3}$  Torr over a temperature range of  $1900$  to  $2600^\circ\text{K}$ .

6) Oxidation reactions of various metals, such as tungsten, tantalum, etc., will be studied at low pressures and high temperatures in the presence and absence of other gases such as nitrogen and halogens.

#### D. Electronic and Magnetic Properties

##### 1. Structure Sensitive Electrical and Magnetic Properties of Materials

Earl R. Parker and Victor F. Zackay

The property of resistanceless conduction, known as "superconductivity," is dependent both on composition and structure. The critical temperature is largely determined by composition and crystal structure and is generally insensitive to defect structure, while the current carrying capacity and critical field are strongly influenced by structural defects of both the microstructural and the atomic types.

Current program interest includes the following:

1) Compounds with the Al<sub>5</sub> (or β-tungsten) crystal structure have the highest critical temperatures of any known superconductors. The critical temperature of the following (as yet unevaluated) metastable Al<sub>5</sub> compounds is being determined: V<sub>3</sub>Al, Ta<sub>3</sub>Au, (Nb,V)<sub>3</sub>Si, and Nb<sub>3</sub>Pb.

2) The critical temperature of compounds with the Al<sub>5</sub> structure usually decreases with increasing deviation from the ideal stoichiometry A<sub>3</sub>B. In the system Mo-Tc, however, an Al<sub>5</sub> structure, perhaps (A,B)<sub>3</sub>B, exists at the approximate composition 50% Mo, 50% Tc. It has a reported transition temperature of 15°K. Further recent theoretical prediction by Leo Brewer indicates that the Al<sub>5</sub> structure should be stable in the ternary system, Mo-Tc-Nb. Studies are being made of the relation of the critical temperature to composition for the binary and ternary systems.

3) The variation of the superconducting transition temperature in the Nb-N-C system is being studied as a function of composition and nitriding pressure.

4) Although compounds having the β-Mn structure have not been extensively investigated, it has been assumed that this structure is not a favorable one for superconductivity. However, current studies of the Al<sub>5</sub> structure of intermetallics and the B1 structure of the metal carbides suggested to us that compounds of the β-Mn structure, especially ternary systems containing nonmetals, would be good superconductors. We have found that the compound Mo<sub>3</sub>Al<sub>2</sub>C and Nb<sub>3</sub>Al<sub>2</sub>C are superconductors with critical temperatures in excess of 10°K.

##### 2. Electronic Properties of Materials

Ira P. Pratt

The specific properties of materials that are directly attributable to conduction electron density, bound electron density (those under the Fermi surface), and electron excitational levels, are being examined on a semi-classical basis. An attempt will be made to extend a.c. relationships describing resistivity and complex permeability to include Larmor frequency in a static magnetic field, and perhaps to include description of the normal to diamagnetic transition associated with superconductors.

Photo-excitation in nonmetals by ultraviolet photons is being experimentally studied to gain information on electron trapping and metastable excitation levels.

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Contract Title: BASIC RESEARCH IN THE METALS AND CERAMICS  
DIVISION

Investigators: John Frye, Director, Metals and Ceramics  
Division and Staff

Scope of Work: A. Crystal Physics

1. Crystal Growth

G. W. Clark, C. B. Finch, S. D. Fulkerson, O. C. Kopp, and A. T. Chapman

The purpose of this program is to study the growth processes of crystals of high-temperature materials, to develop methods of growing such crystals with improved size and quality, to produce crystals of new materials of theoretical or practical value, and to supply crystals for study of physical properties. Growth methods employed include from molten-salt solvents, from supercritical aqueous systems, by material transport, by traveling-solvent techniques, and by the general flame-fusion method. Crystals produced have been used in investigations of neutron irradiation, magnetic properties, electron-spin resonance, and optical absorption.

Beryllium oxide crystals have been grown in different shapes from different alkali tungstate melts at about 1200°C. Addition of 1%  $B_2O_3$  to  $Li_2O \cdot 2WO_3$  increased the growth rate of high-quality thorium oxide crystals at 1200°C from this solvent about tenfold (to 0.02 mm/hr). Thorium oxide crystals are being grown doped with rare earths for study of electron spin resonance and optical absorption of the rare-earth ions.

Several members of a family of new rare-earth germanomolybdate crystals have been synthesized. These have a tetragonal crystal structure like sheelite ( $CaWO_4$ ) and a formula  $R_2GeMoO_8$ , where R represents a lanthanide. These crystals are quite transparent, strongly paramagnetic, and distinctly anisotropic magnetically.

The optical absorption spectra, the optical Faraday effect, and the temperature dependence of the magnetic susceptibility of these crystals are being studied. By analysis of neutron diffraction data,  $\text{Er}_2\text{GeMoO}_8$  was found to remain paramagnetic down to liquid helium temperature.

The allotropic behavior of thorium silicate ( $\text{ThSiO}_4$ ) has been resolved. The transformation is so sluggish that the transformation temperature and even its existence have been in doubt. From solutions in alkali ditungstates and dimolybdates, we could crystallize only thorite (tetragonal) below  $1225 \pm 10^\circ\text{C}$  and only huttonite (monoclinic) above this temperature. This technique should be useful for studying allotropy in other systems with sluggish transformations.

Supercritical ammonia is being investigated as a hydrothermal-type crystal-growing medium.

## B. Physical Metallurgy

### 1. Theory of Alloying

J. O. Betterton, D. S. Easton, and G. V. Czjzek

This program is aimed at an experimental investigation of the properties of metals that are fundamental to the systematic prediction of alloy properties. Measurements include low-temperature galvanomagnetic properties (which provide information on Fermi surfaces), low-temperature specific heats, superconducting transition temperatures, superconducting specific heats, and Mössbauer effect. Particular emphasis is placed on the early transition elements, Zr, Nb, Mo, Hf, Ta, and W, which have found use in the technologies of nuclear energy, space, high temperatures, and superconductivity.

Low-temperature specific heats have been measured for the hexagonal alloy systems Ti-Zr, Hf-Zr, Zr-Sc, and Zr-dilute Nb and interpreted in terms of the electron configurations of the elements and their effects on the electron energy bands in the alloys. Measurements will be extended to more concentrated Zr-Nb alloys, including the body-centered cubic phase, and to the Zr-Mo and Ti-Sc systems. We also expect to measure low-temperature electrical resistivity of several of these systems to more fully define the metallurgical states of the alloys.

Low-temperature galvanomagnetic properties of single-crystal tungsten, beryllium, and zirconium have been measured and interpreted in terms of the Fermi surfaces of these metals. Further work is planned on beryllium, zirconium, niobium, and tantalum. An ultra-high-vacuum ( $10^{-10}$  torr) furnace is being prepared to produce exceptionally pure specimens for this program.

Mössbauer measurements have been made of the structure of grain boundaries in nickel and the precipitation of cobalt in aluminum. The technique will be extended to investigation of localized magnetic moments in superconductors.

A magnet-calorimeter combination has been built to determine the specific heats of metals in the superconducting state in magnetic fields up to 42,000 gauss.

## 2. Relation of Properties to Structure of Metals

C. J. McHargue, R. E. Reed, and R. A. Vandermeer

The purpose of this program is to study the principles dictating atom rearrangements brought about in metals by thermal treatment, mechanical deformation, phase transformations, and irradiation.

Dislocation dynamics is being studied for the body-centered cubic metals. Present studies are concerned with the effects of such variables as minor impurities, alloy additions, temperature, and strain rate on dislocation velocities in niobium. The results are being correlated with the dislocation substructure shown by electron microscopy.

Preferred orientation studies are primarily concerned with correlation of annealing textures of aluminum specimens with prior history. Studies of non-steady-state migration of grain boundaries suggest that vacancies affect migration rates. Further studies of this type and studies of interactions of grain boundaries with impurities will be pursued.

Studies of niobium annealing have demonstrated that twin intersections nucleate recrystallization and have revealed the relative mobilities of various kinds of twin and grain boundaries. These studies will be continued and annealing kinetics will be correlated with different types of dislocation substructure.

The determination of energies of formation and migration of point defects in body-centered cubic metals is under consideration.

### 3. Metallurgy of Superconducting Materials

M. L. Picklesimer, G. R. Love, and J. A. Wheeler

Superconducting electromagnets capable of field strengths up to 60,000 gauss are commercially available, and single wire tests indicate that much higher field strengths are attainable. Metallurgical variables such as heat treatment during and after fabrication, phase morphology and composition, fabrication procedures, and impurity levels have profound effects on the ability of superconducting materials to carry electrical current in a magnetic field. This program is established to investigate the effects of these variables on the superconducting properties of alloys in order that better understanding will lead to superconductors with optimum properties.

A new laboratory has been occupied. Included are a glove-box facility for handling technetium and a high-vacuum ( $10^{-5}$  torr) furnace capable of over 2000°C for preparing, studying, and heat-treating the refractory alloys that have good superconducting properties.

The transformation kinetics of niobium-zirconium alloys containing 30 to 50% Zr have been measured. The measurements will be extended to the range 15 to 30% when a homogenization method now being sought is obtained. Some measurements of superconducting characteristics have been made on alloys with known metallurgical history in this system, but this work is being deferred while a method is being sought for joining superconductors to normal conductors without excessive contact-resistance heating of the superconductor near the joint. Transformation kinetics and morphologies are also under study for uranium alloyed with 25 to 50% Zr.

Preparations are under way for studies of phase equilibrium, transformation kinetics, and superconductivity in technetium-base alloys containing zirconium, niobium, and molybdenum.

### 4. Deformation in Crystalline Solids

R. O. Williams and R. J. Arsenault

The purpose of this program is to investigate the rate-controlling processes that occur during deformation of metals and alloys and the nature of the internal changes brought about by this deformation.

The calorimetric measurement of energy storage during deformation has been extended to single-crystal copper by development of an extremely sensitive calorimetric technique. An isothermal calorimeter is being developed to measure the energy released during recovery and recrystallization.

An extensive investigation is under way on the deformation of body-centered cubic metals, devoted to measurement of activation energies and activation volumes as functions of stress, temperature, and strain rate. Alpha iron has been analyzed completely, and work has started on tantalum alloys. The mechanism of deformation of body-centered cubic metals has been analyzed theoretically by calculation of the energy to nucleate a double kink for external stresses up to the Peierls stress, and a direct measurement of the Peierls stress will be attempted.

The yield drop has been studied as a function of strain rate and temperature for tantalum, Cu-16 at. % Al, and Ag-6 at. % Al, representing three types of dislocation locking. The activation volumes determined from the strain-rate dependence of the yield drop and from differential strain-rate tests agree well. The temperature dependence of the yield drop strikingly resembles that of the ratio of the temperature to the activation volume. As a result of these observations, we conclude that the yield-drop phenomenon is related to the multiplication of dislocations during their motion.

A theoretical analysis of the interaction between slow moving dislocations and carbon atoms in iron predicts a maximum dragging force at a very low strain rate, and the associated activation energy should be that for diffusion of carbon in iron, namely about 20 kcal/mole. In agreement with this, we have found that the activation energy for low-temperature deformation of various iron-carbon alloys does peak at this value for a strain rate that is independent of carbon content.

## C. Ceramics Research

### 1. Sintering Studies

C. S. Morgan and C. S. Yust

High-temperature materials are often fabricated by sintering of compacted powders. This program is directed toward an understanding of the mechanism of sintering, particularly in materials

such as thorium oxide and uranium dioxide that have the fluorite structure. The properties observed include densification rates, grain growth, pore closure, creep, and diffusion.

The dominant role of plastic flow in the initial sintering of thorium oxide has been demonstrated for a variety of conditions including the incorporation of small quantities of calcium oxide, which aids sintering. Like thorium oxide,  $UO_{2+x}$  (O/U from 2.03 to 2.25) probably sinters by plastic flow, since in the range 900 to 1400°C the sintering rate increased with temperature disproportionately more than do diffusion rates.

Compressive creep studies have shown that the high-temperature plasticity of thorium oxide is increased by calcium oxide addition and further by a ternary addition of aluminum oxide. The rate of grain growth, which is important in the final stages of sintering, has been measured for the dioxides of thorium and cerium. Further measurements of creep and grain growth in materials with the fluorite structure are contemplated.

#### D. Structure and Physical Properties of Liquids and Solids

##### 1. Physical Property Studies

D. L. McElroy, W. Fulkerson, T. G. Kollie, and J. P. Moore

The object of this program is the improved understanding of heat transfer in all kinds of solids by careful measurements on selected materials over a broad range of temperature. The ultimate objective is the prediction of thermal conductivity from either first principles or more easily measured properties. Important to this purpose is the improvement of experimental accuracy and the extension of measurements to higher temperatures.

With the improved radial heat flow apparatus, the thermal conductivity of uranium dioxide has been measured from -57 to 1100°C, of type CGB graphite from 50 to 1000°C, and of Armco iron from 100 to 1000°C. Uranium dioxide behaved as a typical ceramic material that is well above its Debye temperature, exhibiting a linear temperature dependence of the thermal resistivity from 200 to 1100°C. The graphite, measured perpendicular to the extrusion direction, showed from 50 to 1000°C a linear thermal resistivity with negligible electronic contribution. In iron, which is a widely used standard for thermal conductivity measurements, the improved accuracy permitted observation of several features not previously observed, such

as the drop in thermal conductivity at  $912^{\circ}\text{C}$ , the allotropic transformation temperature. Measurements of electrical conductivity on the same materials have enabled separation of the electronic and lattice components of the thermal conductivity. Thermocouples with better stability are needed and being sought to permit measurements at higher temperatures. Measurements on electron-beam melted iron and lithium fluoride are planned.

The thermal comparator has been improved in accuracy and used with  $\text{ThS}$  and  $\text{UO}_{2-x}$ ; the latter showed 15% greater thermal conductivity than the stoichiometric oxide. To supplement the comparator a low-temperature longitudinal heat-flow apparatus has been built and is being modified to permit measurements to  $200^{\circ}\text{C}$ .

The direct-heating apparatus, which should permit simultaneous measurements of a number of physical properties to  $2000^{\circ}\text{C}$ , has been assembled and is being tested.

## 2. Spectroscopy of Ionic Media

G. P. Smith, C. R. Boston, and H. W. Joy

This program is a fundamental investigation of the relations between the electronic states and geometrical structure of matter. The major part of the effort is an experimental investigation, principally by optical spectroscopy, of ions primarily in molten salts but supplementally in crystalline salts and molecular liquids. In a complementary theoretical investigation, techniques are being developed for the quantum mechanical calculation of electronic states of atoms, molecules, and crystals.

A study of the effect of surrounding cations on the spectrum of nitrate ion is nearing completion. Copper(II) ions in dilute solution in molten chlorides with large cations were found to be tetrahedrally coordinated to chloride ions with little distortion. Nickel(II) ions in molten  $\text{LiF-NaF-KF}$  eutectic were octahedrally coordinated to fluoride ions. Electronic transitions in the complexes  $\text{NiCl}_4^{2-}$ ,  $\text{NiBr}_4^{2-}$ , and  $\text{NiI}_4^{2-}$  have been measured in high-temperature media and related to modern theoretical models. The rate of oxidation of  $\text{NO}_2^-$  in molten perchlorates was measured spectrophotometrically. Spectroscopic studies of the interactions between ions in different oxidation states of posttransition metals is continuing; recent measurements have been on the  $\text{Bi}^+ - \text{Bi}^{3+}$  and  $\text{Pb}^+ - \text{Pb}^{2+}$  interactions.

The high-temperature spectrophotometer has been demonstrated capable of operation to above 2000°C, although the specimen holder available at present limits measurements to 1450°C. At this temperature the broadening of absorption bands in ruby by lattice vibrations was studied.

Computer programs have been developed for deriving theoretical parameters from spectral data, for calculating electronic states of F-centers in crystals, and for calculating quantum mechanical wave functions from first principles. Improved wave functions have been calculated for  $H_2^+$ , He, Li, C, and  $CH_3^-$ .

### 3. Fundamental Research in X-Ray Diffraction

H. L. Yakel, B. S. Borie, and C. J. Sparks, Jr.

This program is concerned with the use of x-ray diffraction for the study of average crystalline structures and the variations from these average structures that arise from imperfections. In this way, the effort is divided into two areas: the determination of the structure of new materials and the study of changes that are made in crystal structure by such processes as deformation and irradiation.

Single crystals of beryllium oxide, grown at high temperature from molten mixtures of metal oxides, have been examined by x-ray diffraction after irradiation at various temperatures to fast neutron doses ranging from  $1 \times 10^{20}$  to  $4 \times 10^{21}$  neutrons/cm<sup>2</sup>. At temperatures near 100°C, when the dose reached about  $5 \times 10^{20}$  neutrons/cm<sup>2</sup>, the irradiation debris was distributed in agglomerates of 10 to 100 defects each, which affected the scattering of x rays by the crystal lattice in a characteristic manner. Above 650°C, the agglomerates were much larger, and the crystal fractured. Above 1000°C, much of the damage was annealed out, but some swelling persisted. This study should soon be completed, and similar studies of other materials will follow.

The x-ray diffraction study of very thin (20 to 400 Å) films formed on single crystal copper by oxidation has continued. X-ray diffraction characterizes the structure of these films in terms of lattice parameter, mosaic spread, relative amounts of different orientations, strain gradients through the films, and impurity effects. Study of oxide films grown on the different surfaces of copper has led to a model that explains the oxidation rate anisotropy among the 311, 110, 111, and 100 faces of copper in terms of lattice registry and imperfections.

In a continuing effort at determining structures of new materials, progress has been made with  $\text{LuMnO}_3$ -type compounds, compounds between beryllium oxide and other oxides, iron-substituted aluminosilicates, rare-earth germanomolybdates, and rare earth titanates.

## E. Chemical Properties of Solids

### 1. Reactions at Metal Surfaces

J. V. Cathcart, R. E. Pawel, and G. F. Petersen

The general purpose of this program is the investigation of the fundamental processes involved in the oxidation of metals. The principal direction of approach is the study of factors affecting the protectiveness of oxide films on metals, particularly the strain in the film and in the underlying metal.

The study of thin oxide films on copper is continuing. By x-ray diffraction, the structure of the film on several faces of single-crystal copper has been determined. The rate of oxidation could be related to disregistry that results in the cuprous oxide lattice from epitaxial stresses. Impurities have been found to change the rate of oxidation in either direction, and these changes parallel the effects of these impurities on oxide lattice disregistry.

When tantalum or niobium oxidizes, oxygen dissolves in the metal creating rather large stresses. The study of this internal oxidation has been aided by the discovery that a layer of anodic amorphous oxide on the metal does not prevent oxidation but actually improves the observation of precipitation of the sub-surface oxide. Although the anodic film is quite inert, it is readily stripped. This has led to a sensitive sectioning technique for use in diffusion measurements; successive very thin sections of the metals can be removed for analysis by alternate anodizing and stripping. This technique has made possible demonstration of anomalously slow near-surface diffusion by uniquely sensitive measurements of diffusion rates in niobium and tantalum. Study of the oxidation of these metals is continuing. Included are properties of oxide films in place and stripped, comparison of the structure and properties of anodic and thermally formed films, and the solution of oxygen in the metals.

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**Contract Title:** BASIC RESEARCH IN THE SOLID STATE DIVISION

**Investigators:** D. S. Billington, Director; J. H. Crawford, Jr., and  
M. K. Wilkinson, Associate Directors, Solid State  
Division and staff

**Scope of Work:**

The motivation for this research lies in the desire and the need to understand the effect of lattice defects on the behavior of solids. The ability to identify the role of each type of defect in determining solid behavior and to be able to calculate its influence in a quantitative fashion is of importance not only for the basic knowledge of solids revealed thereby but for technology in general, and has a most important bearing on the reactor programs of the AEC. The complexity of the experimental techniques and the sophistication of the experiments are easily understood in view of the large number of possible defects and their agglomerations plus the uncertain knowledge of the mechanism of the interaction between different defects.

Substantial progress has been made, but it is becoming increasingly clear that extremely sophisticated approaches are now required to achieve precise numerical constants. In order to make our approach more sophisticated we are expanding the scope of our effort to employ new and valuable techniques and have organized our effort under four main headings. The details of our diversified approach are given immediately following.

A. Irradiation Effects on Metals  
F. W. Young, Jr.

The purpose of the studies of irradiation effects on metals is twofold: investigations of the effects of irradiation on the physical and chemical properties of metals, and the use of irradiation as a tool in investigations of the mechanisms of production of defects and the properties of the defects. Since many of the physical and chemical properties of metals are directly related to defect structures, these studies have immediate significance in the practical aspects of reactor materials, but emphasis here is placed on a fundamental understanding of the problems rather than an investigation of reactor materials, per se.

1. Effects of Low Temperature Irradiation

R. R. Coltman, C. E. Klabunde

The mobility of point defects in metals at temperatures below room temperature, resulting in the annealing of irradiation damage at low temperatures, has necessitated the study of the production and subsequent annealing of defects at temperatures as low as 3.5°K. To detect the defects and to determine their effects on the metals, electrical resistivity, dimension changes, stored energy and yield stress are measured. The damage is now studied from fast or thermal neutrons independently.

2. Anelasticity

D. O. Thompson, V.K. Paré, P. DeNee

To investigate the interaction of defects introduced by irradiation with the dislocations present in metal crystals, the anelasticity of copper crystals as a function of irradiation is being studied. This has proved to be an extremely sensitive method for the detection of the interaction between dislocations and irradiation-produced defects, and consequently is used for investigation at low irradiation levels. This research is concerned with the motion of defects to dislocations, the subsequent interactions between defects and with the dislocations, and the effect of the defects on the mobility of the dislocations in connection with mechanical properties. Also, the nonlinear elastic behavior of metals is being investigated.

3. Role of Defects in Surface Reactions

L. H. Jenkins, U. Bertocci, L. D. Hulet, F. W. Young, Jr.

The role of crystal defects in the chemical reactivity of metal surfaces is under study. Since there is little basic information on this subject, primary emphasis has been on investigations of the role of dislocations on chemical reactivity; a similar investigation on point defects will follow, and finally the results of these investigations will be used to interpret the effects of reactor irradiation on chemical reactivity. The process of dissolution of copper crystals in aqueous solutions is being investigated, using electrochemical techniques in connection with optical and electron microscope examination of the surfaces.

4. Growth and Characterization of Nearly Perfect Crystals

F. W. Young, Jr.

The growth, preparation and characterization of nearly perfect metal crystals is necessary to the successful completion of the several studies. Accordingly, methods of crystal growth and preparation are being developed. Among the methods of characterization being used, particular attention is placed on X-ray topographic techniques. The X-ray methods are compared with etch pit techniques. Also, the mechanical properties of the nearly perfect crystals are under investigation.

5. Sputtering

A. L. Southern, M. T. Robinson

As another method of investigating the elementary processes occurring during irradiation damage, the bombardment of metal surfaces with ions of moderate energy is being studied. This process results in the ejection (sputtering) of atoms from the surface.

The quantities of interest include the number of target atoms removed per incident ion (yield), the charge, mass and velocity distribution of the ejected particles and their ejection directions with respect to the crystal lattice (ejection patterns).

B. Defect Structures in Nonmetals  
J. H. Crawford, Jr.

Introduction of defects by corpuscular as well as ionizing radiation has been a valuable technique for the investigation of interactions between lattice defects and between lattice defects and impurity atoms in crystalline solids. In fact, results of such studies have formed contributions to the knowledge of the defect solid state as important as direct studies of the nature of radiation damage. In the present program both types of approaches are given nearly equal emphasis; i.e., radiation effects are studied because of the intrinsic interest in the processes by which radiation creates defects and because of the opportunity they afford for understanding interactions between lattice imperfections. The former aspect is important to an appreciation of the service limitations of nonmetallic materials used in radiation environments while the latter is basic to an understanding of the influence of defects upon the behavior of nonmetallic solids.

This program in the past has emphasized the influence of lattice defects on the electronic behavior of semiconductors and more recently has been extended to include electronic defects in ionic crystals (color centers, trapped charge, etc.). In both instances the direction of progress has led to the area of interactions between defects. The present range of materials of interest includes both the extreme examples of valence type, namely elemental semiconductors which are purely covalent, and alkali halides which are predominantly ionic. In addition to these certain semiconducting materials which exhibit a mixture of covalent and ionic binding, such as CdS, CdTe, and ZnS, come under consideration.

1. Radiation Effects in Semiconductors

J. W. Cleland, J. C. Pigg, R. O. Chester

The radiation sensitivity of the electrical properties of silicon has been determined for a wide range of neutron energy (0.2 to 14.1 MeV) using a variety of nuclear reactions. There is a monotonic increase in the apparent electron removal rate of n-type silicon at least up to 4 MeV. This is in marked contrast to n-type germanium, for which the removal rate saturates for neutron energies higher than 0.7 MeV. The result suggests that p-type disordered regions and their associated extensive space-charge zones are not nearly so important a factor in neutron irradiated silicon as compared to germanium.

Isochronal annealing studies of germanium irradiated with  $\text{Co}^{60}$   $\gamma$ -rays at 77°K are being extended to include arsenic-doped as well as antimony-doped specimens. Both exhibit an annealing stage near 130°K, which accounts for only 2 to 4 percent recovery in electron concentration but 40 to 50 percent recovery of the reciprocal mobility change. This annealing stage is attributed to the motion of vacancies to donor sites forming vacancy-donor complexes. Pairing with the donors does not necessarily alter the concentration of deep acceptors but will reduce the carrier scattering drastically through the mutual cancellation of charge on defects and donors.

Progress in studies of radiation effects in cadmium sulfide is being made. It has been shown that defects introduced predominantly in the sulfide sublattice, produced by  $\text{Co}^{60}$   $\gamma$ -irradiation, result in an increase in electron concentration and defects in the cadmium sublattice caused by  $(n, \gamma)$  recoil upon thermal neutron capture decrease the electron concentration. Studies of optical absorption spectra and luminescence of irradiated cadmium sulfide are being continued and will be extended to cadmium telluride.

## 2. Color Center Studies

E. Sonder, W. A. Sibley, R. B. Murray

Investigations on the radiation coloring efficiency in crystals of potassium chloride, grown in different ways and receiving certain types of treatments, are being continued. The conclusion has been reached that trace impurities, of the order of 1 atom in  $10^6$  atoms, could affect the colorability. By adding certain specific impurities (Pb, Ca, Sr) to a "pure" KCl sample, we have now found that as little as 1 Pb atom in  $10^7$  atoms affects the colorability. The effect is particularly marked at low intensities of irradiation. A number of preliminary experiments were performed to see whether the dependence of radiation F-center production on trace impurity and on intensity, found in the vicinity of room temperature, was also present at  $80^\circ\text{K}$ . In agreement with other investigators, little or no intensity dependence was found. However, there were indications that lead impurities could change the colorability significantly.

The coloration properties of crystals which had been deformed and heat treated suggest that the easy formation of color centers after deformation of a crystal is due to debris left behind by dislocation intersection and not the dislocations themselves, as had been previously supposed by some investigations. It has been determined that heat treating a deformed sample to  $450^\circ\text{C}$  for 10 minutes anneals out the dislocation debris and, therefore, the easy coloration. Another interesting aspect of this work, which ties in well with that mentioned in the previous paragraph, is that samples obtained from various suppliers have different amounts of easy coloration for the same amount of deformation. This could be due to the action of trace impurities acting as electron or hole traps, or it could be that the dislocation networks (and hence the deformation properties) vary with crystals prepared in different ways.

It has become apparent that temperature changes of only a few degrees can cause the coloration of samples to change significantly. Moreover, a radiation destruction of color centers has been observed after long, heavy electron irradiations and subsequent decreases of radiation intensity. This radiation destruction is highly temperature sensitive. Therefore, equipment to control sample temperature in the gamma sources has been developed. One of the sample chambers in the gamma source can now be held constant to  $\pm 1^\circ\text{C}$ .

In connection with a theoretical study of the excited states of the F-center, a careful study of the K-band in KCl was undertaken. The K-band which lies at the short wavelength side of the F-band is postulated to be associated with a transition of the F-center electron. Careful measurements of the band shape and location in both irradiated and additively colored KCl at both  $4^\circ$  and  $77^\circ\text{K}$  have been made.

### 3. Light Scattering Studies

W. A. Sibley

The light scattering and dislocation etch pit results show that crystals obtained from different places vary in both trace impurity content and dislocation arrays. Moreover, it has been found from polarizability measurements that certain optically anisotropic impurities, such as  $\text{BO}_2^-$  and  $\text{OCN}^-$ , precipitate at dislocations and give rise to an orientational dependence of the light scattering for the crystals.

### 4. Luminescence Studies

R. B. Murray, C. T. Butler

Color centers and thermoluminescence in irradiated potassium iodide activated with thallium are being examined. These studies relate to a research program devoted to electron-self-trapped hole recombination processes and a fundamental study of scintillation.

Techniques have been developed for employing the emission of luminescence from certain impurity ions in KCl as an analytical tool to estimate impurity concentrations. This is particularly effective for certain of the transition metal impurities which are good activators in the alkali halide host.

In order to better understand the nature of carrier recombination and trapping processes in the alkali halides, a continuing program of studies of the intrinsic luminescence in KCl near  $430 \text{ m}\mu$  was begun. The studies include ultraviolet excitation and triboluminescence (excitation by deformation), and both irradiated and additively colored KCl are found to exhibit this intrinsic luminescence under ultraviolet excitation, but only irradiated materials show luminescence under deformation.

### C. Theory and Computations

D. K. Holmes

The over-all purposes of the theoretical group are (1) the development and extension of theories of the solid state, especially in regard to those problems arising from radiation damage and (2) the application of current theories to experimental results. The second purpose is in response to the need for theoretical help on the part of experimentalists. This type of activity, on a day-to-day basis, is most important for the advancement of understanding, but is difficult to evaluate because, while discussions with the experimentalists are very time consuming, they do not often lead to specific reportable or publishable results. While explicit benefits from consultation with experimental groups are difficult to document or plan ahead, it is felt that the time and effort expended, which may amount to 25 or 50 percent of the group activities, are well justified in terms of aid provided to progress on the experimental fronts. In some cases, such as the electron displacement cross sections and kinetics of radiation enhanced diffusion, collaboration with experimental programs leads to more extended calculations which can be presented in completed form.

The first, main purpose, however, is to develop theory in such a way that radiation effects may be better understood, and that the resultant information may be used to improve the theories of solid state in general. It is difficult to summarize the

scope of present work in this area, since there are a number of studies under way whose subject is dependent on the particular background and interests of the investigator. Further, it is one of the advantages of theory that it is adaptable; programs may be rapidly begun or halted as new problems arise. At present, one of the main areas of interest is the annealing of radiation damage. Through isochronal and isothermal annealing studies, it is possible to obtain information as to the energies of motion of defects produced by the irradiation. The theoretical part of such studies consists of calculations of annealing results to be expected on the basis of a number of models of defect motion, annihilation and trapping. Comparison with experimental results, then, may allow the identification of the temperature range of mobility of a particular defect. If a given model is successful, it may also be possible to estimate the range of interaction of defects with other defects, with impurity atoms, and with dislocation lines. These values are, of course, of fundamental importance in the lattice theory of defects, their associated lattice strains and their electronic structure.

Besides the production and lattice nature of the damage from irradiation, theory must also consider the effects of the defects produced on the properties of the solid. This is an enormously varied area of research because of the number of types of defects, the large number of solid state properties to be considered, and the different types of solids, metals, semiconductors, ionic crystals, etc., in which the given defect may have vastly different effects.

Some of the theoretical work involves the use of large capacity computing machines. In line with this, the scope of the theoretical work has been somewhat increased by use of computing machines to generate tables of functions of importance to solid state physics, in general, and to radiation damage in particular.

1. Radiation-Enhanced Diffusion  
J. H. Barrett

To aid in interpreting experiments on short-range order produced in alloys by enhanced diffusion due to irradiation, calculations are being made of the concentration of defects to be expected during irradiation. The dependence of enhanced diffusion on the defect production rate, temperature, defect motion energies, and sink density has been obtained in various approximations.

2. Diffusionless Self-Annealing  
D. K. Holmes, G. Leibfried

The fraction of defects which will annihilate in a vacancy-interstitial cluster by purely mechanical attraction (no thermally activated process considered) has been calculated. Using Monte Carlo methods this effect has been shown to be important in random arrays. Recently, it has been shown that the calculation can be done analytically to a certain approximation. The analytical approach allows the study of spatial correlations of defects during the annihilation process.

3. Theory of Atom Ejection Patterns  
M. T. Robinson

Studies of the ejection of metal atoms from the surface of a crystal after the deposition of a certain amount of kinetic energy on one internal atom have been

conducted using a simplified, hard sphere model of the lattice. The primary and its progeny are followed through a series of collisions, using the CDC 1604A computer, culminating in the build-up of a theoretical ejection pattern which depends on the crystal geometry, the chosen size of the hard spheres, and the point of origin and energy of the primary. It has been found that very short rows of atoms (2 to 6 atoms long) are sufficient to give spot patterns similar to those observed experimentally.

#### 4. Range Studies

M. T. Robinson, O. S. Oen

The computer studies of the ranges of atoms (having energies from 1 to 100 keV) in amorphous solids have been completed. It has been found that the shapes of the calculated range distributions using the Thomas-Fermi-Firsov potential are in close agreement with those found by experiment.

#### 5. Electron Displacement Cross Sections

O. S. Oen

Displacement cross sections for the production of primary knock-on atoms produced by fast electrons have been calculated for 18 representative heavy elements of the periodic table, using the Mott scattering series. All cases were done for electron energies ranging from threshold to 10 MeV together with several typical displacement thresholds. Displacement cross sections for the whole cascade using the Kinchin and Pease model were also computed for all of the above cases.

#### 6. The Pseudo-Potential and Liquid Metals

W. H. Young, A. Meyer

The pseudo-potential technique has been used to calculate the electrical resistivity of liquid alkali metals. The results are encouragingly in agreement with experiment.

#### 7. The Paramagnetic Scattering of Neutrons by Conduction Electrons

H. D. Dietze

The paramagnetic scattering of neutrons by conduction electrons was calculated. It was found that small angle scattering and simple conditions exist if the ratio of the wavelength of the electrons at the Fermi surface to the wavelength of the neutrons is great in comparison with unity but still small in comparison with the ratio of the mass of the neutron to that of the electron. If experiments are feasible, it should be possible to obtain information about the shape of the Fermi surface.

#### 8. Electronic Structure of Lattice Defects in Ionic Crystals

R. F. Wood

A program for the calculation of the properties (especially optical) of lattice defects in ionic crystals has been developed. Thus far the program has yielded results which compare reasonably well with experimental data on the electronic structure of the M-center in LiCl and LiF. Some success has also been achieved in calculation of the higher excited states of the F center in LiCl.

9. The Magnetic After-Effect  
H. D. Dietze

The theory of the magnetic after-effect at high temperatures in iron with a few percent of silicon, due to the diffusion of vacancies into the domain walls, has been extended to the case of continuously distributed sources and sinks for the vacancies. The theory is in good agreement with the experimental results.

10. Computation  
E. J. Lee

Computer programming and analytical calculations have been performed for (a) radiation enhanced diffusion, (b) etch pit profiles, and (c) function tabulation.

D. Fundamental Investigations in Crystal Physics  
M. K. Wilkinson

The purpose of this program is the investigation of fundamental properties of solids by various experimental techniques applicable to crystal physics. These research activities, which include superconductivity and low temperature physics, magnetic resonance, electron microscopy, X-ray diffraction, and neutron scattering, are being utilized to obtain a better understanding of the physical processes that occur in crystal lattices. Particular emphasis is placed on the manner in which lattice imperfections influence the behavior of solids and on the dynamical properties of crystal lattices.

1. Superconductivity and Low Temperature Physics  
S. T. Sekula, R. H. Kernohan

Much developmental effort is presently concerned with the use of high field superconductors in solenoidal magnets for various purposes, which include plasma physics, bubble chambers, maser accelerators, and simple high field solenoids. Although some theoretical and experimental progress has been made recently to provide a better understanding of superconducting alloys, many interesting aspects are not understood. Investigations are being performed in this program to determine the behavior of superconducting alloys with and without appreciable defects. Defects are being introduced by irradiation and controlled cold work so that the nature of these interactions can be determined, and both the intermediate state and the mixed state of the superconductors are being investigated.

2. Thermal Conductivity and Calorimetry  
W. T. Berg, D. Walton

Research in low temperature thermal conductivity and adiabatic calorimetry has been initiated to give independent information on crystalline defects and lattice vibrations in solids and also to allow investigations of the interaction between the defects and vibrations. Information on the latter interaction can apparently be obtained only by very careful examination of the low temperature lattice thermal conductivity.

### 3. Magnetic Resonance

R. A. Weeks, M. M. Abraham

The electron spin resonance technique is used to develop atomic scale models for those defects in single crystal insulators that are paramagnetic and to investigate the effect of crystalline electric fields in splitting the energy levels of magnetic atoms. The correlation of the paramagnetic defects with optical absorption bands and luminescent bands can aid in understanding some of the defect structures and processes in such crystals. A determination of the crystalline field effects provides information on the magnetic properties of atoms in particular environments within a host crystal and also on the degree of covalent bonding between the atoms of that crystal. Some of the interesting crystals being studied in this program have not previously been available in adequate size, but they are now being grown at ORNL with control of both impurities and crystal uniformity.

### 4. Electron Microscopy

T. S. Noggle

Electron microscope studies of irradiated thin films and foils lead to direct observations of some of the features of radiation effects in solids and thereby contribute to the more detailed understanding of radiation damage. Particular emphasis is being directed toward the study of fission damage in solids with the goal of relating the observable damage with specific interactions between the fragments and the solid. The role of the material parameters on the detailed structure of the induced damage is being evaluated. Thin films and foils of metals and alloys are also being studied after irradiation with other energetic particles to obtain direct observation of radiation damage and evidence of interactions between radiation-induced defects and other structural defects.

### 5. X-ray Diffraction

R. Nicklow, F.A. Sherrill, F.W. Young, Jr.

X-ray diffraction experiments provide numerous methods for the investigations of imperfections in crystals, and special techniques have been refined for this purpose. These techniques include Lang topographical methods with normal and Bormann transmission, double-crystal spectrometry, and the Berg-Barrett method of image contrast in the reflected beam. This program is strongly oriented toward an understanding of the defects in metal crystals, and is closely associated with the metals research group which has undertaken the growth of very pure metal crystals with a low dislocation density. A detailed investigation of the anomalous X-ray transmission through nearly perfect copper crystals is in progress.

### 6. Neutron Scattering

M. K. Wilkinson, H. G. Smith

Neutron scattering investigations are being utilized in a more comprehensive study in those areas that are not being adequately studied at the present time. The intense neutron beams available at the ORR and HFIR provide excellent opportunities to initiate studies of small angle scattering with long wavelength neutrons and studies of inelastic neutron scattering. The small angle scattering experiments can provide

important information on the number and disposition of defects created by fast neutron bombardment, while the inelastic scattering experiments provide information on atomic and molecular energy levels and on phonon and magnon interactions in solids. The inelastic scattering of neutrons is the only method which gives direct information on certain dynamical properties of crystal lattices. Neutron diffraction studies of magnetic and chemical properties are coordinated with programs in the Physics and Chemistry Divisions.

E. Research and Development on Pure Materials  
J. H. Crawford, Jr., J. W. Cleland

The purpose of this program is to develop the necessary techniques for the production of research quality materials needed in selected areas of materials research. Progress in understanding of the fundamental properties and ultimate range of properties in many materials demands research specimens with a high degree of purity and perfection. Extensive studies on materials (usually single crystal) of controlled perfection are required to provide a complete analysis of the properties and capabilities of those materials of immediate and long-range interest to investigators at this laboratory, other AEC installations, and AEC contractors.

The choice of materials for consideration in the program has been made, for the most part, on the basis of the potential gain to a fundamental understanding of solids that should be realized through an intensive investigation of a given material by a number of research groups. Most materials of commercial interest, e.g., the elemental semiconductors, are not being actively considered since reasonable specimens are usually available from commercial suppliers. Certain research materials that have not been investigated previously are being produced, and techniques of purification and crystal growth have had to be extended to these.

Information concerning the physical properties and availability of high purity, research quality specimens has also been difficult to obtain; therefore, as a part of this program, the Research Materials Information Center has been established to collect and provide information on the initial purification, crystal growth, final analysis, and characterization of research materials. Improvement in the dissemination of information on research materials has already been of great benefit to the research community, and it is felt that an accurate, up-to-date listing of available materials has served to eliminate a large amount of duplication of effort incurred in attempts to produce materials that are already available. A simultaneous listing of those research materials that are not available but are desired by various investigators is also being compiled.

1. Materials Preparation in the Metals and Ceramics Division

G. W. Clark, C. B. Finch, A. P. Chapman, O. C. Kopp, S. D. Fulkerson

More than 20 high temperature, inorganic compounds have been synthesized in single crystal form in the Metals and Ceramics Division from molten salt solvents, supercritical aqueous systems, traveling solvent techniques, and by the general flame-fusion method. Some of these crystals have been used in neutron irradiation, magnetic, electron spin resonance, and optical absorption investigations. Earlier experiments on the growth of BeO from  $\text{Li}_2\text{O}\cdot 2\text{WO}_3$  in the range of 1200°C have now been extended and conditions necessary

for growth of pyramids, prisms, or plates of hexagonal symmetry have been established. The growth rate of  $\text{ThO}_2$  from  $\text{Li}_2\text{O}\cdot 2\text{WO}_3$  melts was increased at  $1200^\circ\text{C}$  about tenfold by the addition of 1 wt percent  $\text{B}_2\text{O}_3$ . The present growth rate is 0.02 mm/hr, and the crystals are of good quality.  $\text{ThO}_2$  crystals doped with rare-earth ions have also been grown. These crystals are valuable in optical and electron spin resonance investigations of rare-earth ions in crystalline fields of known symmetry.

A family of new rare-earth germanomolybdate crystals, which may prove useful in magneto-optical devices, have been synthesized. They have a tetragonal crystal structure like that of scheelite ( $\text{CaWO}_4$ ) and a formula  $\text{R}_2\text{GeMoO}_8$ , where R represents a lanthanide. These crystals transmit visible light, are strongly paramagnetic, and have large magneto-crystalline anisotropy. Studies of the temperature dependence of the magnetic susceptibility, the optical absorption spectra, and Faraday rotation are in progress. Neutron diffraction studies reveal that  $\text{Er}_2\text{GeMoO}_8$  remains paramagnetic down to  $4^\circ\text{K}$ .

## 2. Materials Preparation in the Reactor Chemistry Division

R. E. Thoma, C. F. Weaver, R. G. Ross, A. J. Singh

Four single crystals of lithium fluoride weighing  $\sim 300$  g each and containing 79.28, 69.24, 50.77, and 87.60 at. percent  $\text{Li}^7$  were produced in the Reactor Chemistry Division. As a result of refinements made in the purification procedures, the crystals were of extraordinarily high purity, i.e., divalent cation contamination of less than 30 parts per billion.

From zone-melting experiments on  $\text{LiF}$ , separation coefficients for several metal fluoride contaminants were measured using both horizontal and vertical zone refining techniques. Values of the separation coefficients measured ranged from  $< 0.1$  for sodium and calcium to 0.2 to 0.3 for Mn and to 0.7 to 0.8 for Mg. Initial experiments were conducted using the Stockbarger technique to grow single crystals of terbium metal.

A high temperature ( $1600^\circ\text{C}$ ) Stockbarger furnace was built and tested; its first use will be in the growth of  $\text{CaF}_2$  crystals.

Very pure potassium fluoride was prepared by sublimation from a melt containing  $\text{UF}_4$ . The  $\text{UF}_4$  served to precipitate contaminant KOH as  $\text{UO}_2$ . Crystals sublimed from this melt contained 50 ppm oxygen as oxide, roughly half that present in the best materials previously available. Very pure  $\text{ZrF}_4$  was also prepared using a multiple-sublimation procedure; crystals obtained with this method contained less than 100 ppm metal contaminants and 150 ppm oxygen.

A method was demonstrated for the production of very high purity  $\text{BeO}$ , via solvent extraction with acetylacetone. The total quantity of blended and dried precursor hydroxide produced during the investigation was equivalent to 2100 g of  $\text{BeO}$  of 99.998 percent purity.

The vapor-crystal equilibrium system of  $\text{Bi}_2\text{Se}_3$  has been determined by controlled selenium vapor pressure experiments at elevated temperatures and activation energy results indicate that bismuth diffusion to the surface is the predominant effect. The magnetic susceptibility of good quality single crystals of  $\text{Cu}_2\text{O}$  has been determined,

and preliminary experiments indicate a reasonable correlation between the paramagnetic ion contribution and the excess oxygen concentration.

3. Materials Preparation in the Solid State Division  
O. E. Schow, C. T. Butler, J. R. Russell

Experiments are being conducted in the Solid State Division in an effort to improve the size of hexagonal cinnabar (HgS) crystals over those previously obtained by vapor deposition techniques. Purification by fractional sublimation has been conducted and several alternative methods of crystal growth are being investigated.

A preliminary study has been made in the Solid State Division of the problems of growing single crystals of CdTe, and several ingots of about 100 grams weight have been made from reagent grade starting materials.

A semi-clean room was established in which to grow the KCl single crystals produced in the Solid State Division. As a result of this and other improvements, the purity of the KCl crystals routinely grown now exceeds that of available commercial crystals. Large single crystals weighing over 200 grams have been supplied to several groups at ORNL and elsewhere for experimentation. Some of the crystals have been retained for careful analyses by the various techniques available at ORNL. Several very sensitive analytical methods have been developed or become available during the past year. One result of a separate research program in the Solid State Division is that it is now possible to analyze the KCl crystals for lead, to an accuracy of a few parts per billion, by a simple and inexpensive optical technique.

4. Research Materials Information Center  
T. F. Connolly

The Research Materials Information Center now has a coded microfilm collection of information (data sheets, reports, papers, and abstracts) of about 7000 references, dating back to 1957. Materials science centers and private and commercial laboratories are cooperating in forwarding current information, including preprints, to the Center. Mail and telephone requests, about two or three per day, are being routinely answered. Visitors have used the retrieval machine profitably for individual searches and the information center has been used to provide preliminary and current information in the preparation of surveys and project organizations. The first aperiodic bulletin, including survey articles on the growth and evaluation of ionic crystals and listings of both available and desired materials, has been issued.

Recent Publications:

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M. A. Breazeale and D. O. Thompson, "Finite-Amplitude Ultrasonic Waves in Aluminum," Appl. Phys. Letters 3, 77 (1963).

D. L. McDonald, "Low Temperature Irradiation of Beryllium Oxide," Appl. Phys. Letters 2, 175 (1963).

- F. W. Young, Jr., and L. D. Hulet, "On the Role of Crystal Imperfections in the Chemical Reactivity of Copper Surfaces," Metal Surfaces, edited by W. D. Robertson and N. A. Gjostein (The American Society for Metals, 1963), p. 375.
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- W. A. Sibley, "Light Scattering in Alkali Halide Single Crystals," Phys. Rev. 132, 2065 (1963).
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- D. K. Holmes, "Radiation Damage in Solids," to be published in Proceedings of the Summer School of Physics, Herceg Novi, Yugoslavia, September 1963.

- D. K. Holmes, "Range Calculations and Channeling," Proceedings of the Solid State Physics Summer School, Mol, Belgium, August 1963 (in press: North Holland Publishing Company).
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- M. T. Robinson and O. S. Oen, "Computer Studies of the Slowing Down of Energetic Atoms in Solids," Phys. Rev. 132, 2385 (1963).
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- H.-D. Dietze, "Theory of Coercive Force for Randomly Distributed Lattice Defects and Precipitations," Phys. kondens. Materie 2, 117 (1964).
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- M. J. Smith, " $\text{Co}^{60}$   $\gamma$ -Radiation Induced Defects in  $\text{Bi}_2\text{Te}_3$ ," *J. Appl. Phys.* 34, 2879 (1963).

PART II  
OFFSITE RESEARCH



Contractor: Alabama, University of, University, Alabama

Contract Number: AT(40-1)-3090

Present Contract Term: February 15, 1964 through February 14, 1965

Cost to AEC: \$26,750

Contract Title: F-SHELL TRANSITION STUDIES

Investigators: E. H. Carlson

Scope of Work:

The interactions between f-shell transition ions in non-metallic crystals are being studied. A search for magnetic ordered states at low temperatures is underway in the rare earth halides isomorphic to  $\text{LaCl}_3$ . Both nuclear magnetic resonance and static susceptibility techniques are being used. A search for pair spectra in diluted (with  $\text{LaX}_3$ ) crystals is being carried out by electron spin resonance. A measurement of heat conductance vs. magnetic field will be undertaken, probably in a laser-type crystal (in order to obtain near perfection in the lattice), in the temperature region 2-20°K. This will be of interest in regard to spin-phonon scattering.

Contractor: Andrews University, Berrien Springs, Michigan

Contract Number: AT(11-1)-972

Present Contract Term: June 1, 1964 through May 31, 1965

Cost to AEC: \$14,500

Contract Title: PHYSICAL PROPERTIES OF SEPARATED METALLIC ISOTOPES

Investigators: Donald D. Snyder

Scope of Work:

There appear to be phase transitions in lithium metal at about  $80^{\circ}\text{K}$  and at about  $150^{\circ}\text{K}$ , the latter being one of the second kind. Isotopic mass is used as a parameter to study these transitions by measuring Young's modulus and the coefficient of linear thermal expansion as a function of temperature (liquid-helium temperature to room temperature). The lower-temperature transition affects the coefficient of thermal expansion as expected, but the higher-temperature one does not. Both transitions are observed in the Young's modulus measurements. X-ray studies of lattice constants will be used to corroborate the macroscopic measurements of the thermal coefficient of expansion in the same temperature range.

Extension of the techniques to other isotopically-enriched samples is planned.

Paul W. McDaniel, Director  
Division of Research

W. F. Shuely, Metallurgy and Materials  
Programs, Division of Research

**NEW CONTACT - UNIVERSITY OF ARIZONA - (EMRICK)**

The simplest defect process in a solid is the motion of a single vacancy from one lattice site to another. This event is the fundamental step in self diffusion and is involved in other solid state processes. However, it has proven experimentally difficult to measure in a direct fashion the important parameters in this process: the activation volume and activation energy. So far, this has been approached by the technique of quenching in a supersaturated concentration of vacancies and measuring the kinetics of their removal on annealing by following the change in resistivity. The problem arises in that with decreasing temperature, single vacancies tend to associate to form stable di- and tri-vacancy clusters which greatly complicate the annealing kinetics. With the techniques available heretofore, it has been necessary to conduct the annealing experiments at the lower temperatures where the kinetics of annealing are slow enough to follow but, where they are complicated by the association reaction.

Prof. Emrick of the University of Arizona proposes a new experimental technique which would permit measurement of annealing kinetics in a temperature range sufficiently high that the point defects would not associate but would migrate to pre-existing sinks for annihilation. This requires extremely rapid heat up to and quench from the annealing temperature, precise and rapid temperature control and resistivity measurement. Emrick has constructed and tested a prototype apparatus in which the quenched sample is held in a reference bath temperature throughout and is heated to the annealing temperature by a shaped electrical pulse. The feasibility of the technique was satisfactorily demonstrated.

Emrick proposes support for himself and two graduate students to develop this apparatus to the necessary degree of accuracy and to use it to determine the migration energies and lifetimes of vacancies in gold, platinum, and aluminum. It is proposed to study the effects of pre-straining on lifetimes and to investigate the feasibility of introducing pressure as an applied variable in order to measure as the pressure derivative of activation free energy. Emrick has had considerable experience in high pressure techniques and in measuring properties of samples under pressure.

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The proposal has been reviewed by Jackson and Baebener (AKL), Koehler (U. of Ill.), and Balluffi (Cornell), all of whom are currently deeply involved in studies of point defect processes. All agree that the problem is timely and important. Jackson and Baebener give their unqualified recommendation. Koehler also recommends support but warns that the value of the work will depend on whether or not sufficient accuracy can be achieved. Balluffi did not feel able to give an unbiased review since he "has been thinking about carrying out work with exactly the same objectives" and because he believes he will have a better technique than that described by Barick. He also mentioned that Koehler was trying a similar experiment but I note that Koehler was silent on this and did recommend support.

Because of Balluffi's accomplishments, it is impossible to discard his statements but because his only negative assertion was a matter of opinion, I judge that the total review was in support of performing the proposed research.

Prof. Barick was a graduate student of Professor Lazarus at Illinois, a point greatly in his favor. Also, Balluffi attested to Barick's capability. I assume through their acquaintance while both were at Illinois.

The total proposed budget is \$36,060. The U. of Arizona will contribute \$15,855 and they request \$20,205 from the AEC. Included in the total is \$1,090 in capital equipment which the U. of Arizona plans to make part of their contribution.

This is a very good proposal, it is of interest to the AEC and the budget is commensurate with the work proposed. I recommend that a contract be written as proposed with title to equipment vested in the contractor in consideration of his contribution.

Prof. Barick is principal investigator on no other Government contract.

He is employed as a senior scientist during the summer on Texnikova's contract. But he told me by phone on 1/12/65 that he would leave that position if this proposal is supported.

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**Contract:** Arizona, University of, Tucson, Arizona

**Contract Number:** AT(11-1)-1041

**Present Contract Term:** June 1, 1964 through May 31, 1965

**Cost to AEC:** \$53,335

**Contract Title:** IMPURITY DIFFUSION IN SOLIDS

**Investigators:** Carl T. Tomizuka

**Scope of Work:**

Objective of this project is to measure the pressure effect and the temperature effect on the rate of diffusion of various impurities in solids.

Reason for this project is that a great deal can still be learned concerning the nature and behavior of vacancies in solids, especially the interaction of vacancies with impurities.

Procedure to be employed are the standard radioactive tracer-sectioning technique, ionic conductivity measurement and Mössbauer spectroscopy all performed at various temperatures and at high pressure.

Test Objects will be gold single crystals, gold-silver alloys, silver chloride, copper single crystals, alpha-brass and sodium chloride doped with Co 57.

Accomplishments to date include the determination of diffusion activation energies for various impurities in copper, completion of the pressure effect measurement of the ionic conductivity in silver chloride, preliminary determination of the pressure effect on the self-diffusion rates in gold and gold-silver alloy and the development of a new chemical sectioning technique to extend the measurable range of diffusion coefficients down to  $10^{-16}$  cm<sup>2</sup>/sec.

**Recent Publications:**

D.L. Styris and C.T. Tomizuka, Anomalous Diffusion Rate for Small Penetration Distance in Copper, Journl Appl. Phys. 34, 1001 (1963).

C.T. Tomizuka, Effect of Hydrostatic Pressure on the Rate of Atomic Movement in Noble Metals, J. Phys. Soc. Japan, 18 Suppl. II, 228 (1963).

Contractor: Arkansas, University of, Fayetteville, Arkansas

Contract Number: AT(40-1)-2096

Present Contract Term: November 1, 1963 through October 31, 1964

Cost to AEC: \$26,456

Contract Title: STUDY OF STRUCTURE OF LIQUIDS BY X-RAY DIFFRACTION

Investigators: P. C. Sharrah and R. F. Kruh

Scope of Work:

A specially built  $\theta - \theta$  diffractometer is being used to study the structure of liquids by x-ray diffraction. Systems currently being investigated include alkali metals, the system lithium-mercury, aqueous and acetone solutions of transition metal halides, carbon halides, liquid ammonia, and aqueous solutions of isopolymolybdates.

Recent Publications:

R. F. Kruh and C. L. Standley, "An X-Ray Diffraction Study of Aqueous Zinc Chloride Solutions," Inorg. Chem. 1, (1962) p. 94

R. F. Kruh, "Diffraction Studies of the Structure of Liquids," Chem. Rev. 62, (1962) p. 319

R. F. Kruh, G. T. Clayton, Charles Head, Glenn Sandlin, "The Structure of Liquid Mercury," Phys. Rev. 129, (1963), p. 1479

Contractor:                    Atomics International, A Division of North American Aviation, Inc., Canoga Park, California

Contract Number:               AT(11-1)-Gen-8

Present Contract Term:        July 1, 1963 through June 30, 1964 (Fiscal year 1964)

Cost to AEC:                   \$286,000.

Contract Title:                SOLID STATE PHYSICS AND DEFECT PROPERTIES

Investigators:                 A. Sosin, A. Anderman, W. Bauer, F.H. Eisen, K. Garr, D.W. Keefer, H.H. Neely.

Scope of Work:

It is the objective of this project to study the production of defects in crystalline solids and to attain an understanding of their structure, their interactions with each other and with impurities and dislocations, their effect on the physical properties of solids, and their recovery kinetics. Emphasis is placed on achieving a basic description both of the defects themselves and their subsequent consequences on physical properties by performing experiments which relate most directly to such a description. For this reason, electron irradiation experiments have been emphasized constantly. The desirability of this technique is evidenced by the increasing activity in this area. Nevertheless, related experiments, involving other techniques and theoretical approaches, are used when appropriate.

#### A. Radiation Effects in Metals

##### 1. Electron Irradiation of Gold W. Bauer and A. Sosin

An intensive study of the production and recovery of point defects in gold after electron irradiation at low temperatures has been completed. No indication of a recovery stage involving long range migration is observed below Stage III (240° to 340°K). The last 55% of this stage is characterized by second order annealing kinetics with an activation energy of  $0.80 \pm 0.04$  eV. The minimum energy required for displacement has been established as 34-36 eV. The characteristics of the production of damage as a function of electron energy combined with the recovery characteristics indicate that only one form of interstitial is created by displacement below 2 MeV and that this form is created in directions close to  $\langle 100 \rangle$  directions.

The results of this study have been written in three consecutive articles and submitted for publication. More preliminary studies have been made on the effects of impurities on the recovery following irradiation. The materials used were 99.999% pure gold, 99.99% pure gold and gold + 0.1 atomic % copper. The influence of the impurities on Stages I and II is considerable.

## 2. Electron Irradiation of Platinum

W. Bauer

The recovery following electron irradiation of platinum has been studied in detail, particularly in the Stages III and IV region. Platinum is somewhat unique among the metals in that Stage IV, studied following quenching by other investigators, has been well established as due to the migration of single vacancies with a migration energy of 1.36 eV. The results of the post-irradiation recovery studies yields the same energy. Thus, Stage III should be most easily identified as not due to any vacancy-type migration. Unfortunately, Stage III appears to be more complex than hoped for, complicating the interpretation.

## 3. Electron Irradiation of Copper Alloys

H.H. Neely and A. Sosin

In addition to the studies of recovery in a variety of copper alloys previously conducted but not yet reported, a detail study has been completed in a series of copper + gold alloy, with up to 1.0 atomic % gold. The results--activation energies, types of kinetics, effect of solute concentration-- have been analyzed for details concerning the nature of the interaction between interstitials and solute atoms.

In general, three new recovery stages are produced by the presence of over-sized substitutional impurities. The impurities investigated are gold, silver, aluminum, zinc, gallium, and nickel. One undersized impurity - beryllium - has also been studied but the recovery spectrum here is more complex. The interaction between these substitutional atoms and an interstitial defect appear to be based on elastic distortions of the lattice, due to atomic size effects, and electrostatic interaction, due to valence differences between solute and solvent atoms (including the interstitial atom).

## 4. Electron Irradiation of Aluminum Alloys

K. Garr and A. Sosin

Following up previous studies on two aluminum alloys (0.1 atomic % Zn and Cu), a series of aluminum alloys has been prepared for irradiation and initial studies near 4°K have been made.

## 5. Electron Irradiation of BCC Metals

K. Garr, D.W. Keefer and A. Sosin

Fabrication, annealing, and mounting procedures for molybdenum, iron, and tungsten have been developed. The sample wire, procured in high purity from commercial sources, is attached to a standard type holder by spot welding. Initial difficulties here have been obviated by welding in an argon atmosphere. The wires are then annealed resistively in a low temperature cryostat specially constructed for this purpose. The design of the cryostat allows different types of annealing treatments, such as in vacuum or controlled atmosphere. With such techniques, samples with reasonably favorable resistivity ratios have been obtained. Initial irradiations have been performed.

## 6. Electron Irradiation of Thin Metal Single Crystals

A. Sosin and K. Garr

The studies of the effects of crystallographic orientation in copper have been completed and a report written. Efforts are being made to fabricate iron and gold single crystals for similar experiments. In iron, efforts are being made to use iron whiskers or to grow alpha-iron single crystal foils from the gamma phase. In gold, three methods are being explored. The first is grain coarsening. Preliminary encouraging results have been obtained in this method. The Bridgeman technique (growth from the melt) is also being attempted in which the sample thickness is 0.001 in. and therefore, immediately available for irradiation, or 0.005 in., in which case electrolytic polishing will be required.

## 7. Continuous Annealing

A. Sosin, W. Bauer, and H.H. Neely

A particularly detailed study of the recovery of resistivity in electron-irradiated copper was made in Stage I, with the resolution of approximately about 12 substages. The resolution of substages is controlled by the fineness in the temperature scale at which data points are obtained in the isochronal techniques used. To obviate this difficulty, a continuous annealing technique has been developed; preliminary measurements are encouraging. If successful, this technique will be used for a variety of metals.

## 8. Dislocation Pinning in Gold

D.W. Keefer

Quenching measurements on a Au modulus sample have been completed. The specimen was quenched from 830°K to 20°K in situ. This treatment increased the resonant frequency somewhat, indicating that some vacancies were present on dislocations after the quench. Subsequent isochronal annealing yielded a pinning stage between 280 and 340°K, precisely the temperature range over which a pinning stage occurs

following electron irradiation. These results confirm the suggestion made in the previous report that vacancy migration in Au occurs between 280 and 340°K. This is also in agreement with results obtained by resistivity measurements in this laboratory.

In the quenching studies, depinning begins at about 420°K. Thus, the depinning observed in irradiated Au between 340 and 550°K is a dual process. The early part of the stage is due to interstitials; that above 420°K can be attributed to vacancies. This has been confirmed in depinning studies made on a heavily irradiated specimen; the two-step nature of the stage is clearly visible.

## 9. Dislocation Pinning in Copper

D.W. Keefer and A. Sosin

Low temperature dislocation pinning studies have shown that Stage III in copper has an activation energy of 0.60 eV and Stage IV, about 1.1 eV. This agrees with previous workers using different experiments. These values and the relative importances of Stage I and III as a function of electron energy are compatible with the two-interstitial model of post-irradiation recovery.

## 10. Point Defect Relaxations

D.W. Keefer

The purpose of this project is to study the effect of low temperature irradiation on low frequency ( $\sim 1$  cps) internal friction at 77°K and above. Particular attention is to be given to possible effects resulting from motion of the split interstitial-type defect. Work on the cryostat for this study is continuing. Mounting and alignment of the sample has been successfully carried out, and the optical system is in place.

## B. Radiation Effects in Semiconductors

F.H. Eisen

Previous studies of radiation damage in InSb have established that this material has an exceptionally low value of threshold displacement energy. Post-irradiation recovery studies after electron irradiation have disclosed a spectrum of recovery stages, nominally composed of six stages, in which the position of the lower two stages--the predominant stages--depend sensitively on the electrical parameters of the material, i.e., the type and concentration of carriers.

A model has now been constructed which explains the Stage II recovery in InSb following electron irradiation. In this model, indium vacancies migrate about two steps, then recombine with the previously ejected indium atom which resides in one of two possible interstitial sites. This model explains the doublet nature of Stage II, the first order character of each of the substages, the observed changes in carrier concentration, the relative magnitude of each substage and the difference in damage rates between (111) and (1 $\bar{1}\bar{1}$ )-oriented samples.

## C. Theoretical

A. Anderman and A. Sosin

An IBM 7094 digital computer program to simulate radiation damage events and defect configurations is being written. The program has a number of unique features incorporated into it. It is the intention to study, in particular, the importance of the nature of the interaction potential on the final results as calculated by the computer and compare directly with the data being obtained in the laboratory.

### Recent Publications:

F.H. Eisen, "Cryostats for Irradiating at 4.2°K," Advances in Cryogenic Engineering 8, (1963).

F.H. Eisen, "Orientation Dependence of Electron Radiation Damage in InSb," Phys. Rev., to be published.

D. Keefer and A. Sosin, "Effect of Low-Temperature Electron Irradiation on Young's Modulus of Pure Cu," Appl. Phys. Letters 3, (1963) p. 185.

D. Keefer and A. Sosin, "Thermal Depinning of Dislocations in Electron-Irradiated Copper," Acta Met., to be published.

D. Keefer and A. Sosin, "Electron Irradiation Hardening of Aluminum," Acta Met., to be published.

W. Bauer and A. Sosin, "Threshold Displacement Energies and Sub-Threshold Displacements in Copper and Gold Near 10°K," J. Appl. Phys. 35 (1964) p. 703.

W. Bauer and A. Sosin, "Point Defect Studies in Gold by Electron Irradiation at Low Temperatures. I. Threshold Displacement Energy and Displacement Cross Section," Phys. Rev., to be published.

W. Bauer and A. Sosin, "Point Defect Studies in Gold by Electron Irradiation at Low Temperatures. II. The Resistivity Recovery Spectrum from 15°K to 240°K," Phys. Rev., to be published.

A. Sosin, "Radiation Effects in Metals at Low Temperatures," Proceedings of the Int'l Conf. on Crystal Lattice Defects, 1962 Conf; J. of the Phys. Society of Japan, 18, Suppl. III.

A. Sosin and L.H. Rachal, "Recovery Study in Pure and Alloyed Aluminum Following Electron Irradiation," Phys. Rev. 130, No. 6, p. 2238-2248.

J.C. Robinson, "A Cryostat Operating from 20°K to 870°K," Review of Scientific Instruments, to be published.

Contractor: Atomics International, A Division of North American Aviation, Inc., Canoga Park, California

Contract Number: AT(11-1)-GEN-8, General Order 9305, Subaccount 5401

Present Contract Term: July 1, 1963 through June 30, 1964 (Fiscal Year 1964)

Cost to AEC: \$201,000

Contract Title: ELECTRONIC STRUCTURE OF METALS AND ALLOYS

Investigators: T. G. Berlincourt and staff

Scope of Work:

This effort is devoted to the acquisition of knowledge regarding the electronic structure of metals and alloys (configuration of electronic energy states in momentum space) and the role of this structure in determining electrical, thermal, magnetic, vibrational, and alloying characteristics. Detailed information on the shape of the Fermi surface is provided by de Haas-van Alphen studies in magnetic fields up to 200 kilogauss, and the density of electronic states at the Fermi level is deduced from low-temperature specific heat measurements. The latter also yield information on lattice vibrational modes and on the interactions involved in superconductivity and magnetic ordering. Further characterization of magnetic interactions is accomplished by means of conventional magnetic susceptibility techniques. Considerable effort is devoted to the exploration of high-field superconductivity with emphasis on thermodynamic and transport characteristics, as well as on the electron energy spectrum as deduced from thin-film electron-tunneling measurements. These experimental investigations are correlated with current theory, and attempts are made to characterize quantitatively the relationship between superconductivity and the normal-state electronic structure.

1. de Haas-van Alphen Effect Studies  
A. C. Thorsen and A. S. Joseph

These investigations have led to a number of advances in the characterization of Fermi surfaces. Detailed measurements (still in progress) on Re have revealed examples of multiple magnetic breakdown similar in many ways to that envisioned theoretically by Pippard [Proc. Roy. Soc. (London) A270, 1 (1962)]. Major progress toward an understanding of the electronic structure in ferromagnets was marked by successful observations of de Haas-van Alphen oscillations in the ferromagnetic metal Ni. Detailed orientation studies have indicated that

one sheet of the Fermi surface in Ni is topologically similar to the major Fermi surface segments observed in the noble metals. Refined measurements on Cu have brought new precision to the determination of the neck orbits in this metal, and, by yielding effective mass data in excellent accord with cyclotron resonance determinations, have resolved an apparent discrepancy of long standing. These same studies provided the first experimental demonstration that spin splitting of the Landau levels leads to a vanishing of the de Haas-van Alphen effect for orientations characterized by an effective mass equal to one half the free electron mass.

## 2. Localized Lattice Modes

J. A. Cape and D. H. Leslie

Low temperature specific heat investigations of Mg (a light host lattice) containing dilute additions of Pb or Cd (heavy impurities) have revealed evidence of localized lattice modes. The results are in good accord with the theoretical prediction that for such a system localized modes, associated with the heavy impurity, should occur in a narrow band of frequencies near the low-frequency end of the phonon spectrum.

## 3. Magnetic Impurities and Superconductivity

R. R. Hake and J. A. Cape

Further characterization of the superconducting and magnetic properties of Ti, Zr, and Hf containing dilute additions of Cr, Mn, Fe, Co, and Gd has been accomplished via magnetoresistance, magnetic susceptibility, and specific heat measurements. This work apparently constitutes the first study of the many different aspects of localized moment behavior in transition-metal-base alloys; the first investigation of the changes in specific heat, resistivity, and magnetic susceptibility due to the insertion of localized moments (Mn) into a transition metal superconductor (Ti-50 at.% Zr); and the first evidence that a localized moment associated with a rare earth ion (Gd) interacts with the conduction electrons in a transition metal (Zr) much more weakly than does a localized moment associated with another transition metal (Mn).

## 4. Thermodynamic Characteristics of Type II Superconductors

R. R. Hake and W. G. Brammer

Calorimetric observations have revealed second-order bulk superconducting transitions and bulk superconducting state energy-gap behavior in high magnetic fields in the low-dislocation-density alloy V-5 at.% Ta. These results constitute powerful evidence in favor of the spatially-uniform negative-surface-energy theories of type II superconductivity. The derivation of entropy, free energy, magnetization, and effective energy gap from the experimental specific heat curves as well as the thermodynamic analysis of volume, compressibility, and thermal expansivity relationships provide valuable insight into the nature of the type II superconductor.

## 5. New Superconducting Phase Nucleation Field

W. J. Tomasch and A. S. Joseph

Torque magnetometer and electron tunneling studies have led to the identification and characterization of a new superconducting phase nucleation field  $H_{C3}$  in both type I and type II superconductors in remarkable quantitative accord with a theory independently proposed by Saint James and de Gennes [Physics Letters 7, 306 (1963)]. The tunneling data provide strong (though not definitive) evidence in support of the sheath-like structure of that theory.

## 6. Delayed Flux Entry in Type II Superconductors

A. S. Joseph and W. J. Tomasch

Studies of the magnetization characteristics of type II superconductors having very smooth surfaces and near-ideal demagnetizing coefficients have revealed gross departures from the near-equilibrium magnetization behavior ordinarily observed for less-perfect conditions. The most striking difference is the delay of bulk magnetic flux penetration to fields sometimes a factor of three greater than the lower critical field, above which, at equilibrium, the bulk of a type II superconductor is threaded by flux. The observed effects may find partial explanation in the surface barrier theory of Bean and Livingston [Phys. Rev. Letters 12, 14 (1964)].

### Recent Publications:

W. J. Tomasch, "Magnetic Field Dependence of Electronic Tunneling in Type II Superconductors," Bull. Am. Phys. Soc. 8, 419 (1963).

R. R. Hake and J. A. Cape, "Superconductivity and Localized Moments in Ticonium," Bull. Am. Phys. Soc. 8, 419 (1963).

T. G. Berlincourt and R. R. Hake, "Superconductivity at High Magnetic Fields," Phys. Rev. 131, 140 (1963).

A. C. Thorsen and A. S. Joseph, "The de Haas-van Alphen Effect in Zirconium," Phys. Rev. 131, 2078 (1963).

A. S. Joseph and A. C. Thorsen, "Magnetic Breakdown in Rhenium," Phys. Rev. Letters 11, 67 (1963).

J. A. Cape, "Superconductivity and Localized Magnetic States in Ti-Mn Alloys," Phys. Rev. 132, 1486 (1963).

A. S. Joseph and A. C. Thorsen, "de Haas-van Alphen Effect in Nickel," Bull. Am. Phys. Soc. 8, 469 (1963).

R. R. Hake, "Thermodynamics of a High-Field Superconductor," Bull. Am. Phys. Soc. 8, 475 (1963).

R. R. Hake, "Thermodynamic Properties of a High-Field Superconductor," *Rev. Mod. Phys.* 36, 124 (1964). Contributed paper at the International Conference on the Science of Superconductivity, Colgate University, August 26-28, 1963.

T. G. Berlincourt, "Type II Superconductivity," *Rev. Mod. Phys.* 36, 19 (1964). Survey paper presented at the International Conference on the Science of Superconductivity, Colgate University, August 26-28, 1963.

T. G. Berlincourt, "High-Magnetic Fields by Means of Superconductors," *British J. Appl. Phys.* 14, 749 (1963). Survey paper presented at the Conference on High Magnetic Fields, their Production and their Application, University of Oxford, July 10-12, 1963.

A. S. Joseph and A. C. Thorsen, "de Haas-van Alphen Effect and Fermi Surface in Rhenium," *Phys. Rev.* 133, A1546 (1964).

A. S. Joseph and A. C. Thorsen, "de Haas-van Alphen Effect and Fermi Surface in Nickel," *Phys. Rev. Letters* 11, 554 (1963).

R. R. Hake and W. G. Brammer, "High-Magnetic-Field Specific Heat of a Low-Dislocation-Density Alloy Superconductor," *Phys. Rev.* 133, A719 (1964).

W. J. Tomasch and A. S. Joseph, "Experimental Evidence for a New Superconducting Phase Nucleation Field in Type II Superconductors," *Phys. Rev. Letters* 12, 148 (1964).

A. S. Joseph and W. J. Tomasch, "Experimental Evidence for Delayed Entry of Flux into a Type II Superconductor," *Phys. Rev. Letters* 12, 219 (1964).

R. R. Hake and J. A. Cape, "Calorimetric Investigation of Localized Magnetic Moments and Superconductivity in Some Alloys of Titanium with Manganese and Cobalt," *Phys. Rev.* (submitted).

W. J. Tomasch, "Electronic Tunneling from Superconducting Pb-Tl Alloy Films in a Magnetic Field," *Bull. Am. Phys. Soc.* 9, 29 (1964).

A. S. Joseph and W. J. Tomasch, "Some Magnetic Properties of Thick-Film Superconducting Pb-Tl Alloys," *Bull. Am. Phys. Soc.* 9, 29 (1964).

A. C. Thorsen and A. S. Joseph, "de Haas-van Alphen Effect in Rhenium," *Bull. Am. Phys. Soc.* 9, 250 (1964).

G. W. Lehman, J. A. Cape, R. E. DeWames, and D. H. Leslie, "Virtual Mode Contribution to Specific Heat of Dilute Mg Alloys," Bull. Am. Phys. Soc. 9, 251 (1964).

W. J. Tomasch and A. S. Joseph, "Experimental Evidence for a New Superconducting Phase Nucleation Field in Type II Superconductors," Bull. Am. Phys. Soc. 9, 252 (1964).

A. S. Joseph and W. J. Tomasch, "Evidence for Surface-Barrier Inhibition of Flux Entry in Type II Superconductors," Bull. Am. Phys. Soc. 9, 252 (1964).

R. R. Hake, "Thermodynamic Properties of a Type II Superconductor," (Invited paper) Bull. Am. Phys. Soc. 9, 257 (1964).

A. S. Joseph and A. C. Thorsen, "Low Field de Haas-van Alphen Effect in Copper," Phys. Rev. (in press).

W. J. Tomasch, "Persistence of Surface Superconductivity beyond  $H_{c2}$  in a Type II Superconductor as Evidenced by Electron Tunneling," Physics Letters (April 1, 1964).

UNITED STATES GOVERNMENT

# Memorandum

TO : Paul W. McDaniel, Director  
Division of Research

DATE: October 28, 1964

FROM : W. F. Shively, Metallurgy and Materials  
Program, Division of Research

SUBJECT: PROPOSED RESEARCH PROGRAM, BATTELLE MEMORIAL INSTITUTE (CLAUER)

R:ADMM:WFS

I have reviewed the attached unsolicited proposal from Battelle entitled, "Correlation of Dislocation Structure with Creep Properties in Refractory Metals." In essence the proposal is to determine the creep activation energy spectrum and stress dependence of creep strain-rate of molybdenum single crystals and correlate these measured properties with the dislocation substructure. The substructure will be determined by transmission electron microscopy of thin sections and etch pitting of the original crystals.

There are three major reasons why this program is appropriate for M&M support:

1. The Commission has a clear interest in the creep properties of refractory metals.
2. The study, as it is planned, will contribute to the development of creep theory since: (a) one of the great weaknesses of present day creep theory is that while we know that substructure development controls the form of the creep curve, we are only able to express the influence of substructure in quantitative terms; and (b) most basic studies of creep have been conducted on h.c.p. and f.c.c. metals. Studies of b.c.c. metals are needed for the development of theory.
3. The metal science group of the Battelle Memorial Institute is uniquely qualified to perform this particular study because of the following combination of factors:
  - a. It has electron-beam crystal-growing facilities and experience in growing refractory metal crystals.
  - b. It has the high-vacuum, high-temperature creep facilities necessary for the experimental program.
  - c. It has an electron microscope laboratory and a staff experienced in transmission electron microscopy.

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- d. Several of the senior staff members in the group where the work will be done are experts in dislocation theory.
- e. The members of this group have good records of basic research in physical metallurgy, thereby providing the proper environment for fundamental research.

Specifically the research will be performed by Mr. A. H. Clauer under the technical direction of Dr. B. A. Wilcox. As a sidelight to the project, it may be noted that Mr. Clauer will use part of the research for his Ph.D. thesis at Ohio State. Mr. Clauer's thesis preceptor is Dr. John Hirth of the Ohio State staff.

This proposal was originally submitted April 1, 1963, under Rosenfeld and Clauer's name. I wrote to the group offering some technical criticism April 5, 1963, and received their rebuttal in a letter of April 19, 1963. The proposal and this correspondence was sent for review to Ruoff (Cornell), McHargue (ORNL), and Thomas (LRL-R). All agree that the proposal is well founded and that the research should be performed. These reviews of a year ago are still satisfactory because so little basic work has been done in this field since that time.

Because of budgetary problems, it was not possible to fund the proposal in FY-64. The proposal was strengthened and brought up to date August 7, 1964. The major changes are that Wilcox will act as supervising scientist and that molybdenum is substituted for columbium as a subject material. Fewer problems are anticipated with molybdenum since it does not have the propensity for contamination of columbium. The professional staff arrangement on the proposed contract was discussed by R. I. Jaffee, Associate Manager in charge of the Metal's Science Group and me, when he first contacted me and said that Clauer wanted to submit a proposal on this work. My opinion was that the proposed experiments appear worthwhile but that some one of the senior staff who has an established record in dislocation research should be associated at least part time with the research in addition to Clauer to insure that the research is performed on a high scientific plane. Originally Rosenfeld took an interest in the project, but because of the delay in funding it, he is no longer available. Dr. B. A. Wilcox joined the Battelle staff in September 1963 after finishing an NSF fellowship at Cambridge where he worked with Hirsch.

Drs. Jaffee and Wilcox visited me at Headquarters on October 30, 1963, to discuss this proposal. I became convinced of Dr. Wilcox's personal enthusiasm for the proposed research. He showed me some results of current research he and Clauer are performing with in-house support which is aiding in the development and refinement of the techniques needed for the proposed research. His biography on page 11 of the proposal shows clearly that his background makes him eminently qualified to guide this research.

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Clauer will devote full time to this activity. Wilcox's responsibilities will be as follows:

- 1/3 Wright-Field, Contract No. AF 33(657)-10363  
"Notch Sensitivity of Refractory Metals"  
4/1/63 - 3/31/64 -- \$25,000  
Anticipated 64/65 support \$50,000  
Coinvestigator with Dr. A. Gilbert
- 1/3 Wright-Field, Contract No. AF 33(615)-1727  
"Elevated Temperature Ductility in W and Mo-TZM Alloy"  
7/1/64 - 9/30/65 -- \$57,400  
Coinvestigator with Dr. A. Gilbert
- 1/6 Battelle Support  
"Elevated Temperature of Creep Properties of Thoriated Nickel"
- 1/6 Our Contract

Dr. Edington would devote about one man-month to the transmission electron microscopy portion of the AEC program.

Because of the merits of the proposal, the unique qualifications of the proposing group, the lack of basic knowledge in the field of the research, and the increasing importance to the Commission of systems involving high temperatures, I recommend that this proposal be accepted and that the contract commence January 1, 1965. To the best of my knowledge, the proposed research does not unnecessarily duplicate work already under way or contemplated by the AEC.

The proposed budget for the first year's operation is \$52,680 of which \$41,430 is requested from the Commission. A total three year program involving \$124,315 of the Commission funds is anticipated. No purchase of capital equipment is involved. I believe that this budget is commensurate with the work proposed and recommend that it be funded accordingly. It is not anticipated that this work will lead to any large scale R&D or production activity.

Scope: The contractor will conduct fundamental study of the creep of body-centered cubic metals with the objective of revealing the influence of substructure on observed creep rate.

Remarks: No AEC funds are to be used to purchase capital equipment without special Headquarters approval.

**Contract:** Battelle Memorial Institute, Columbus, Ohio

**Contract Number:** W-7405-eng-92

**Present Contract Term:** March 1, 1964 through February 28, 1965

**Cost to AEC:** \$26,000

**Contract Title:** THE CHARGE ON INTERSTITIAL IONS IN GROUPS IV-A AND V-A

**Investigators:** P. S. Rudman

**Scope of Work:**

By measuring the rate of interstitial migration in an applied DC electric field the effective interstitial charge in solution in refractory bcc metals will be obtained. Combining these results with additional electrical resistance and magnetic susceptibility measurements, the true interstitial state of ionization in solution will be determined which will be related to interstitial alloying behavior. Electromigration and resistivity studies will be compiled in the Nb-O, Ta-O, Ti-O, and Mo-O systems.

In the past year, the experimental techniques and the apparatus for the electromigration studies, and the interstitial charging and analysis techniques were developed. Preliminary electromigration and resistivity measurements on the Nb-O system were made.

**Contract:** Bausch & Lomb Incorporated, Rochester, New York

**Contract Number:** AT(30-1)-1312

**Present Contract Term:** January 1, 1964 through December 31, 1964

**Cost to AEC:** No-fund Extension

**Contract Title:** IRRADIATION DAMAGE TO GLASS

**Investigators:** N. J. Kreidl

**Scope of Work:**

This research is concerned with the effects of high energy radiation on some of the optical, electrical, and mechanical properties of glasses.  $\text{Co}^{60}$  gamma rays and 1.5 MeV electrons were used. The work at present falls mainly into two categories: effects of radiation on fused silica compressed under high pressure, and effects of radiation on electrical conductivity of various glasses. Work on high pressure effects is being pursued with the tetrahedral device described in the November 1961 report. Pressures up to 100 kilobars can be obtained. The device has been calibrated for pressure; temperature calibration will be completed soon. High temperatures and pressures have been applied to small cylinders of fused silica; the most useful range of pressure and temperature for subsequent radiation studies will be determined. The effects of high pressure on glass melted under oxidizing and reducing conditions is under study. Absorption and density differ according to the atmosphere used. In the conductivity studies, measurements are being carried out on fused silica, lead silicate glass, phosphate glass, and Pyrex. Cycles of measurements on charging and discharging currents have been made which show several distinct relaxation times. These are being correlated with structure when possible.

**Contract:** Brown University, Providence, Rhode Island

**Contract Number:** AT(30-1)-2024

**Present Contract Term:** May 1, 1964 through April 30, 1965

**Cost to AEC:** \$48,177

**Contract Title:** RADIATION DAMAGE STUDIES IN SOLIDS USING THE TECHNIQUES OF ELECTRON-SPIN PARAMAGNETIC RESONANCE AND NUCLEAR MAGNETIC RESONANCE

**Investigators:** Philip J. Bray  
Henry O. Hooper

**Scope of Work:**

Nuclear magnetic resonance (NMR) and electron-spin resonance (ESR) studies will be continued on single crystals of several neutron-irradiated alkali halides to gain information concerning the defect structures in these materials. In order to derive more detailed and specific information from such studies attempts will be made to obtain crystals of lower dislocation content, to neutron irradiate crystals under more controlled conditions through the use of the new Rhode Island Reactor, and to initiate nuclear magnetic-electrical quadropole double resonance experiments. A further study of the production and the properties of the gas and metallic phases created in lithium fluoride under heavy neutron irradiation will be continued and extended to other lithium halides, sodium fluoride and calcium fluoride. The effects of the dislocation content and of thermal annealing upon the growth of the gas and metallic phases will be examined in detail.

Electron-spin paramagnetic resonance studies of  $\alpha$ -irradiated alkali borate glasses, cabal ( $\text{AcO-B}_2\text{O}_3\text{-Al}_2\text{O}_3$ ) glasses and related crystalline compounds will be further investigated at room, liquid nitrogen and liquid helium temperatures. In association with this work on the structure of glasses, a program of the study of paramagnetic ions in glass will be continued. Much effort will be devoted to this work employing both glasses and associated crystalline compounds which have been doped with various paramagnetic ions.

**Recent Publications:**

Sook Lee and P. J. Bray, "Electron-Spin Resonance Studies of Irradiated Glasses Containing Boron," J. Chem. Phys. 39, 2863 (1963).

Contract: Brown University, Providence, Rhode Island

Contract Number: AT(30-1)-2394

Present Contract Term: June 1, 1964 through April 30, 1965

Cost to AEC: \$59,298

Contract Title: A COMBINED MACROSCOPIC AND MICROSCOPIC APPROACH TO THE PROPERTIES OF METALS

Investigators: Joseph Gurland and D. C. Drucker

Scope of Work:

A combined metallurgical and "continuum mechanics" study of the mechanical properties of metals as a function of the microscopic structure is being undertaken. Subjects currently under investigation are:

- 1) The elastic constants of heterogeneous materials.
- 2) The mechanical properties of grain boundaries.
- 3) The variation of mechanical properties in two-phase alloys containing a ductile matrix: yield strength, crack initiation, and ductile rupture.
- 4) The analysis of stresses due to inclusions.
- 5) The fracture strength transition in two-phase alloys.
- 6) The quantitative description and measurement of structural variables.
- 7) The effect of microstructure on the fracture strength and the fracture path of steels.

Recent Publications:

D. Gucer and J. Gurland, "An Application of Fracture Statistics to the Microstructure of Cemented Carbides," Jernkontorets Annaler (Sweden), 147, (1963) p. 4.

J. Gurland and J. Plateau, "The Mechanism of Ductile Rupture of Metals Containing Inclusions," Trans. ASM, 56, (1963) p. 442.

T. T. Wu, "On the Parametrization of the Elastic Moduli of Two-Phase Materials," Technical Report No. 4, October 1963.

Contract: California Institute of Technology, Pasadena California

Contract Number: AT(04-3)-221

Present Contract Term: 1 June 1964 - 31 May 1965

Cost to AEC: \$219,403.46

Contract Title: FUNDAMENTAL STUDIES OF MATERIALS PERTAINING TO NUCLEAR ENGINEERING

Investigators: Pol Duwez, Professor of Materials Science  
R. H. Willens, Assistant Professor of Materials Science  
K. Das Gupta, Senior Research Fellow in Materials Science

Scope of Work:

The main subject of this project is the study of metastable phases in alloys rapidly quenched from the liquid state. These phases are either solid solutions beyond the equilibrium limits, new intermediate crystalline phases which are not found under conventional cooling rates or amorphous alloys. The structure of these alloys are studied by x-ray diffraction, electron-diffraction and electro-microscopy. The physical properties under study include electrical resistivity (from 2.3 K up to the melting point) Hall effect, paramagnetic susceptibility, ferro-magnetic properties (Curie temperature and B-H curves) thermoelectric properties and superconducting properties. Other studies are concerned with the kinetics of transformation of metastable phases and with the mechanism of crystallization of amorphous alloys. The effect of electron irradiation on the devitrification of amorphous phases is in progress. Studies are being made of the band structure of a few selected alloys by means of soft x-ray spectroscopy (emission and absorption).

Recent Publications:

H. L. Luo and Pol Duwez, "Metastable Amorphous Phases in Tellurium Base Alloys," Applied Physics Letters, 2, (1963) p. 21.

W. Klement, Jr., "Hexagonal Close-Packed Structures in Bi-Pb Alloys and the Polymorphism of Lead at High Pressure," J. Chemical Phys., 38 (1963) pp. 298-299.

C. C. Chao, H. L. Luo and P. Duwez, "Cs-Cl Type Compounds in Binary Alloys of Rare-Earth Metals with Gold and Silver," J. Appl. Phys., 34, (1963) pp. 1971-1973.

H. L. Luo and Pol Duwez, "Face-Centered Cubic Cobalt-Rich Solid Solutions in Binary Alloys with Aluminum, Gallium, Silicon, Germanium and Tin," Canadian J. of Physics, 41, (1963) pp. 758-761.

Pol Duwez and R. H. Willens, "Rapid Quenching of Liquid Alloys," Trans. Metal. Soc. AIME, 227, (1963) pp. 362-365.

W. Klement, Jr. and H. L. Luo, "Metastable Solid Solutions in Silver-Platinum Alloys," Trans. Metal. Soc. AIME, 227, (1963) pp. 1253-1254.

W. Klement, Jr., "Solid Solutions in Gold-Cobalt and Copper-Cobalt Alloys," Trans. Metal. Soc. AIME, 227, (1963) pp. 965-970.

Contractor: California Institute of Technology  
Pasadena, California

Contract Number: AT(04-3)-473

Present Contract Term: November 1, 1963 through October 31, 1964

Cost to AEC: \$51,907

Contract Title: A STUDY OF DISLOCATION MOBILITY AND DENSITY IN METALLIC  
CRYSTALS

Investigators: D. S. Wood and T. Vreeland, Jr.

Scope of Work:

An experimental program is under way to measure the relation between dislocation velocity and resolved stress in various metals and under various conditions. Velocities are determined by measuring the displacement of individual dislocation etch pits resulting from the application of a stress pulse. A rapid-load torsional stress machine has been constructed which is capable of applying stress pulses with a rise time of about three microseconds and a minimum duration of  $17 \times 10^{-3}$  seconds.

Present studies of the velocity ( $v$ ) relation using basal dislocations in zinc single crystals yield data fitting the relation:  $v = K(\tau - \tau_0)^n$  where  $\tau$  is the applied resolved shear stress and  $\tau_0$  is the static flow stress. The value of  $n$  ranges from 1 to 1.5. This work is continuing and includes an effort to learn the effect of temperature and density of dislocations threading through the slip plane on the parameters of the velocity-stress relation.

Work has been initiated on the effect of point defects introduced by electron bombardment on the velocity relation in copper and, possibly, aluminum. The techniques are also being applied to yielding in iron-silicon alloys to contribute to the solution of the question whether the factor governing the yielding behavior in bcc metals is Cottrell locking or rates of velocity and multiplication of mobile dislocations.

**Contract:** California, University of, Berkeley, California

**Contract Number:** AT(11-1)-34 #47

**Present Contract Term:** August 1, 1963 through July 31, 1964

**Cost to AEC:** \$50,000

**Contract Title:** MICROWAVE FARADAY ROTATION AND OTHER STUDIES

**Investigators:** Alan M. Portis

**Scope of Work:**

The problems now under investigation are concerned largely with the properties of ordered magnetic materials -- both metals and insulators. We are placing particular emphasis on resonance techniques -- nuclear and electron resonance as well as double resonance, and microwave Faraday rotation. In addition we are equipped to determine crystal structure and to measure static and torsional susceptibility.

The major problems now being studied are summarized below:

1. The ferromagnetic transition in metals. We are using microwave Faraday rotation to measure correlation times near the transition temperature and above.
2. Magnetic properties of dilute alloys. We are attempting to use nuclear-magnetic double resonance in the study of the magnetic properties of dilute alloys.
3. Properties of antiferromagnetic insulators. We are continuing our investigations of crystals of class  $X Mn F_3$ , where X is one of the alkalis. We are currently doing direct nuclear resonance on the Mn-55 nuclei. In addition we are investigating transient magnetization processes in these materials, having completed an exhaustive study of double nuclear-antiferromagnetic resonance.
4. Electrical properties of organic materials. We are initiating a study of the electrical properties of organic materials using microwave Faraday rotation.

**Recent Publications:**

A.M. Portis, G.L. Witt, and A.J. Heeger, "Excitation of Nuclear Resonance Modes in Antiferromagnetic  $K Mn F_3$ ," J. Appl. Phys. 34, (1963) p. 1052.

A.M. Portis, "Low-lying Spin Wave Modes in Ferromagnetic Films," Appl. Phys. Letters 2, (1963) p. 69

**Contract:** California, University of, Berkeley, California

**Contract Number:** AT(11-1)-34 #76

**Present Contract Term:** January 1, 1964 through December 31, 1964

**Cost to AEC:** \$40,000

**Contract Title:** PHONON RESEARCH IN SOLIDS

**Investigators:** Klaus Dransfeld

**Scope of Work:**

The following projects are presently pursued:

1) New Methods for the Excitation of Elastic Surface Waves

2) Hypersonic Waves in Metals: In the microwave frequency range the wavelength of ultrasonic waves becomes shorter than the coherence length over which electron pairs are correlated in superconductors, and shorter than the skin depth in normal metals. Furthermore a new interaction with "helicon waves" is expected. No ultrasonic absorption measurements have been done so far in this interesting frequency region.

3) Far Infrared Absorption in Dielectrics: Between 200 and 2000 micron the absorption of dielectric solids (crystals and glasses) is being measured down to liquid helium temperatures. The temperature dependence at the lowest temperatures is most important for the theoretical understanding of the absorption process.

4) Hypersonic Absorption in Dielectric Crystals: Ultrasonic absorption measurements below 40°K in MgO show a relaxation peak at 13°K which is probably caused by Fe++ impurities, but more experiments are needed. The hypersonic absorption in the alkali halides has never been investigated and is being planned.

5) Raman Scattering of Laser Light by Macromolecules in Solution:

6) Absorption of Hypersonic Waves in Liquids

**Recent Publications:**

Klaus Dransfeld "Kilomegacycle Ultrasonics," Scientific American, Vol. 208, No. 6, (1963) pp. 60-68

Contract: California, University of, Riverside, California

Contract Number: AT(11-1)-34, Project No. 77

Present Contract Term: August 1, 1963 through July 31, 1964

Cost to AEC: \$53,820

Contract Title: ELECTRIC AND MAGNETIC PROPERTIES OF TRANSITION METALS  
AND THEIR COMPOUNDS

Investigators: A. W. Lawson

Scope of Work:

This contract is devoted primarily to the study of the electrical and magnetic properties of the transition metals and their compounds, with particular emphasis on their pressure dependence. During the last year, a study of the conductivity of silver mercuric iodide and copper mercuric iodide has been carried out in an effort to ascertain why in the ordered phases of these compounds, the silver salt is ionic in nature whereas the copper salt is a semiconductor. In addition, the electrical conductivity of  $Ti_2O_3$  and  $V_2O_4$  is being studied as a function of pressure to check Mott's theory<sup>2,3</sup> of the transition from insulating to conducting behavior. A novel apparatus has been constructed to study paramagnetic and ferromagnetic resonance as a function of pressure. Initial data has been obtained on gadolinium, iron and nickel. The resonance frequency is shifted up in iron about 2%/kilobar, no shift is observable in nickel, and is shifted up about 1%/kilobar in Gd with increasing pressure. The line shape changes markedly in iron, narrows in nickel and gadolinium. Experiments as a function of temperature on europium sulfide (EuS) are also in progress. During the coming year, these experiments will be repeated on single crystals and extended to other systems. The conductivity work will also be brought to fruition.

**Contract:** California, University of, Los Angeles, California

**Contract Number:** AT(11-1)-34 #103

**Present Contract Term:** June 1, 1964 through May 31, 1965

**Cost to AEC:** \$38,800

**Contract Title:** SPECTROSCOPIC STUDY OF LATTICE VIBRATIONS IN CRYSTALLINE SOLIDS

**Investigators:** Robert A. Satten

**Scope of Work:**

We are engaged in the study of lattice vibrations of crystals by a number of spectroscopic means, viz. in the far infrared, by Raman effect, and by vibronic spectra involving rare earth and actinide type ions. The latter is a relatively undeveloped means due to difficulties in interpretation, but one we believe will prove to be a very fruitful method. We have already shown some of the possibilities, but many questions remain, particularly concerning the influence of various regions of the Brillouin zone. A far infrared grating spectrograph for the region down to  $50 \text{ cm}^{-1}$  is being constructed using a Perkin Elmer Model 210 monochrometer. Various types of detectors have been or will be tried including Golay, special thermocouples, bolometer, and doped semiconductor types. Raman effect studies on crystals whose lattice vibrations have been studied by means of the vibronic spectra of crystals containing rare earth and actinide type ions will be undertaken. These materials will also be the first we shall examine when the far infrared spectrograph is completed. A calculation of the lattice vibrational frequencies vs k vector (sampling many points in the Brillouin zone) for  $\text{LaCl}_3$  is being programmed on the IBM 7090. Long range monopole and dipole forces including the polarizabilities of the atoms are included, as well as Born-Mayer repulsive forces. The intensities of vibronic bands of salts containing  $\text{UCl}_6^-$  and  $\text{UBr}_6^-$  complexes are being measured and computed as a function of a number of parameters. It is hoped that the parameters can be adjusted to yield agreement with experiment.

**Recent Publications:**

I. Richman, R. A. Satten, and E. Y. Wong, "Lattice Vibrations in  $\text{LaCl}_3$  and  $\text{LaBr}_3$  from Vibronic Spectra", J. Chem. Phys. 39, 1833 (1963).<sup>3</sup>

J. B. Gruber and R. A. Satten, "Analysis of the Electronic Spectrum of Neodymium Ethylsulfate", J. Chem. Phys., 39, 1445 (1963).

Recent Publications: (continued)

C. J. Lenander and E. Y. Wong, "Crystal Field Shielding in  $\text{PrCl}_3$ ",  
J. Chem. Phys. 38, 2750 (1963).

C. J. Lenander, "Parametrized Slater-Modified Hartree-Fock Method  
Applied to Actinide Ions", Phys. Rev. 130, 1033 (1963).

Paul W. McDaniel, Director  
Division of Research

December 1, 1964

Mark C. Wittels, Metallurgy and Materials  
Programs, Division of Research

**NEW CONTRACT WITH THE UNIVERSITY OF CALIFORNIA AT LOS ANGELES (CHESTER)**

This proposal consists of two parts and is entitled "1. Second Sound In Solids, and 2. Electroabsorption Studies in Semiconductors." The research is essentially an experimental study in two fairly new areas of solid state physics in which Professor Chester has already made some progress. In addition to the principal investigator, one post-doctoral fellow and one graduate student are proposed participants this first year.

The first study concerning second sound, is at present only known to exist in liquid helium below  $2.2^{\circ}\text{K}$  and although some efforts to discover the effect in solids have been made over a dozen years or so no success has yet been achieved. Every substance has a critical thermal oscillation frequency,  $f_c$ , below which the phenomenon of second sound apparently does not exist. This critical frequency is zero for liquid helium and is expected to exceed the megacycle per second range for most other materials. It is suggested that the earlier efforts to discover the effect in solids failed because this frequency condition was not recognized in  $\text{Al}_2\text{O}_3$ , where relatively low frequencies of the order of 10 kilocycles per second were employed.

It is proposed to initiate the studies on KCl, which at  $2^{\circ}\text{K}$  should exhibit a critical frequency of approximately 250 kilocycles per second. Both the temperature and frequency range are technologically feasible here. The calculations also indicate that at  $4^{\circ}\text{K}$  quartz requires 30 megacycles per second and diamond about 700 kilocycles per second. These materials might also be candidates.

To pursue these experiments fast thermometry techniques will be employed and it is expected that even if the phenomenon of second sound in solids remains unobservable the development of the techniques will undoubtedly help in other areas of solid state research, particularly with phonon relaxation processes.

At present, part of the cryogenic set-up is ready, KCl crystals have been grown and cleaved, and part of the continuous wave equipment has been assembled. The thermal transmission through several materials will be attempted into the megacycle range at liquid helium temperatures.

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By this effort it is hoped that the present theories on second sound in solids will be thoroughly tested and that high speed thermometry techniques will be highly developed for phonon relaxation studies.

The second area of research involving electroabsorption studies in semiconductors is also a relatively new field which is open for exploitation. The prediction of an electric field effect on the band gap optical absorption edge in semiconductors was originally presented in 1958 by Keldysh (Soviet) and Franz (German). In the experiment suggested here it is proposed to follow the shift in optical absorption in samples subjected to an electric field. Both the field and the incident light wavelength can be varied to secure a wide data area. In addition, the parameters of temperature and crystal orientation can be varied to provide further information. Although this proposed study is definitely one of basic research there are strong technological reasons for pursuing this area. For example if a large change in band edge absorption could be produced under an applied electric field then an avenue would open for efficient solid state light modulators. This would possibly have important significance to advanced laser and communications systems.

One of the important observations already made in electroabsorption phenomena is that there is a strong analogy between electric field and magnetic field characteristics. Both produce a ladder of evenly spaced energy levels and it is important to find whether in the electric field case there is a structure related to the band gap optical absorption charges, as in the well-known magnetosorption case. If so, it is suggested that an oscillatory behavior will result and this will be sought. Professor Chester has already made good progress in developing the electronic techniques for making these important observations.

This proposal has been favorably reviewed by Pohl (Cornell), Callaway (California) and Wannier (Oregon). It should be noted that the latter reviewer demurred on the second sound studies because he felt they were "doomed." The other equally capable reviewers were not so disposed, however, and even felt the investigation was "exciting." I concur with the majority, and even if it were a minority, I would feel that the financial risks were well worth the potential scientific gain.

The budget appears satisfactory and the research is definitely of interest to the AEC. Support is therefore strongly recommended with the following financial arrangements:

AEC Funds	\$61,631
UCLA Funds	28,493 (31 1/2%)
Total	\$90,124

Professor Chester has no federally supported research contracts at present. Title to the equipment should be vested in the University since its contribution exceeds its value.

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Paul W. McDaniel, Director  
Division of Research

December 3, 1964

Mark C. Wittels, Metallurgy and Materials  
Programs, Division of Research

**NEW CONTRACT WITH THE UNIVERSITY OF CALIFORNIA AT LOS ANGELES (CLARK)**

This is a new proposal entitled "Experimental Research in Solid State Physics by Magnetic Resonance Methods," with Professor W. Gilbert Clark as principal investigator, one post-doctoral, and two graduate student participants. By utilizing magnetic resonance techniques as the main tool study is suggested for six interconnected experiments of varying importance and difficulty. These include the construction of a pulsed nuclear resonance apparatus, measurement of the quadrupolar shift of NMR frequencies under an applied uniaxial strain, nuclear polarization with crystal rotation, nuclear resonance in tantalum, nuclear polarization by a dc current, and spectral study of nuclear spin states in the neighborhood of paramagnetic impurities. The principal investigator has already shown good experience and competence in all of these proposed programs.

The pulsed nuclear resonance apparatus will be modified to cover a frequency range of 1-60 Mc, to allow ENDOR and ADRF experiments to be conducted.

Quadrupolar shifts of NMR frequencies under applied uniaxial strains are to be studied under conditions where unwanted line broadening will be removed either through crystal perfection or thermal diffusive motion. The technique should be applicable to a wide variety of materials including alkali halides, intermetallic compounds, and possibly some metals and alloys. In particular, the linear splitting of satellite resonance lines under applied stress will be closely followed to determine the relations between anti-shielding crystal electric field gradients, and nuclear quadrupole moments, all of which are important to nuclear physics as well as solid state physics.

The nuclear polarization through crystal rotation studies can be used, at low temperatures, to reveal the interactions among phonons, electrons, and nuclei in solids. Use of a ferroelectric material whereby the switching of domains through an electric field is suggested as a new technique to replace the crystal rotation method. Previous measurements of nuclear resonance in tantalum revealed a rather broad central resonance that was attributed to sample imperfections. It is hoped that spin-lattice relaxation measurements in tantalum can be performed below 78°K and that

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purier metal can be secured to allow for more accurate relaxation time measurements.

The nuclear polarization by dc current studies are proposed in a continuation of some work already initiated on indium antimonide. In addition the work is to be extended to other materials in which hot electrons can be produced, and to experiments in which the detailed mechanisms for producing nuclear polarization can be deduced.

The last project involving nuclear magnetic spin states will probably involve ENDOR and rotating frame techniques, among others, and will be directed towards dielectric crystals containing paramagnetic impurities. The results of these studies should be closely related to the nuclear polarization experiments.

I have discussed the wide breadth of this proposal with Professor Clark and he has agreed to follow a list of priorities so those areas with the greatest promise will be pushed as the need presents itself. The proposal has received favorable outside review from Knight (California), Portis (California), Silsbee (Cornell), and Watkins (G. E.). The research is definitely in AEC interests and support is recommended as indicated in the budget.

ABC funds	\$66,490
UCLA funds	57,155 (46%)
Total	\$123,645

Professor Clark has no federally supported research contracts at present. Title to the equipment should be vested in the university since its contribution greatly exceeds its value.

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Contractor: Carnegie Institute of Technology, Pittsburgh, Pennsylvania

Contract Number: AT(30-1)-2314

Present Contract Term: January 1, 1964 through December 31, 1964

Cost to AEC: \$11,800

Contract Title: SURFACE DIFFUSION ON METALS

Investigators: Paul G. Shewmon

Scope of Work:

From the experimental results of our grain boundary grooving work on surface diffusion on copper, one would expect that surface must be transporting matter one to several orders of magnitude faster than volume diffusion during the early stages of neck growth in sintering, at comparable high temperatures. However, it is generally agreed in the sintering literature that volume diffusion is the dominant mechanism of matter transport for copper as well as most other metals. It appears that either the sintering literature or the grain boundary grooving literature must be wrong on this point. Since the mathematical analysis used in the grooving work is much more rigorous than that used in the sintering work, the author's feeling is that surface diffusion is really the diffusion mechanism that determines the rate of neck growth in sintering.

To establish the dominant transport mechanism in sintering, we will apply Herring's scaling laws rather than the more commonly used times laws due to Kuczynski. Experimentally, the rate of neck growth is being determined using a line of copper spheres and the electron microscope.

The same sort of analysis indicates that grain boundary diffusion should become dominant in the shrinkage of powders at temperatures below about 3/4 of the melting point. We will also try to check out this prediction, although an unequivocal determination of the mechanism is more difficult here.

Recent Publications:

G. Love and P. G. Shewmon, "Self-Diffusivity of Silver in Twist Boundaries," Acta Met., Vol. 11, 1963, p. 899-906.

Recent Publications: continued

Paul G. Shewmon, "Surface Diffusion from a Point Source," Jnl. Appl. Phys., Vol. 34, No. 4 (Part I), (1963), p. 755-757.

F. R. Winslow and P. G. Shewmon, "Orientation Dependence of the Surface Free Energy of Silver by a New Method," Trans. Met. Soc. AIME, Vol. 227, (1963), p. 1078-1080.

**Contractor:** Carnegie Institute of Technology, Pittsburgh, Pennsylvania

**Contract Number:** AT(30-1)-2360

**Present Contract Term:** March 15, 1964 through October 31, 1964

**Cost to AEC:** \$12,064

**Contract Title:** THERMAL CONDUCTIVITIES OF INORGANIC MELTS

**Investigators:** W. O. Philbrook

**Scope of Work:**

This research has been concerned with the measurement of the thermal conductivity of molten inorganic substances and correlation of the results with the electrical conductivity and other transport properties of the melts. The purpose is to reveal the mechanisms of thermal conduction and to contribute to the knowledge of the structure and properties of these liquids. The substances of immediate interest are those which show semiconductor behavior in the liquid state. Data have been reported for silver and nickel sulfides near the compositions  $\text{Ag}_2\text{S}$  and  $\text{Ni}_2\text{S}_3$ , respectively. Research under way is directed at completion of research on thermal conductivities in the Ag-Te system as a function of temperature and composition across the liquid field on both sides of  $\text{Ag}_2\text{Te}$ . The apparatus used for past studies has been rebuilt with improvements that permit operation at temperatures up to  $1100^\circ\text{C}$  with improved precision over the original model.

**Contract:** Carnegie Institute of Technology, Pittsburgh 13, Pennsylvania

**Contract Number:** AT(30-1)-3001

**Present Contract Term:** May 1, 1964 through April 30, 1965

**Cost to AEC:** \$21,430.

**Contract Title:** THE INTERACTION BETWEEN POINT DEFECTS AND DISLOCATIONS

**Investigators:** Charles L. Bauer

**Scope of Work:**

A number of experiments are in progress that utilize elastic constant and internal friction measurements to investigate some of the structure sensitive properties of crystals. Research to be undertaken during the next contract year is enumerated as follows:

1. The binding energies of Si and Sn atoms to dislocations in dilute Cu alloys will be measured and compared with predicted values.
2. Theoretical work concerning time-dependent internal friction will be continued.
3. Computer studies will be initiated to analyze the theory of dislocation damping.
4. Internal friction and elastic modulus measurements will be made on a number of materials in the temperature region of liquid helium in order to study thermally activated dislocation unpinning.
5. Ultraviolet irradiation studies will be performed on alkali halide single crystals in an attempt to observe dislocation pinning.
6. An investigation will be initiated utilizing dislocation damping techniques to study the effect of chemical impurities and plastic deformation in hard superconductors.

During the last contract year the solute atom-dislocation binding energy in dilute Cu-Ge alloys was experimentally found to be 0.28 eV in good agreement with the predicted value of 0.31 eV. In addition, a detailed study of dislocation damping in dilute Cu-Ge alloys has been completed.

**Contract:** Carnegie Institute of Technology, Pittsburgh 13,  
Pennsylvania

**Contract Number:** AT(30-1)-3033

**Present Contract Term:** April 1, 1964 through March 31, 1965

**Cost to AEC:** \$35,940

**Contract Title:** RADIATION EFFECTS IN SOLIDS

**Investigators:** D. A. Wiegand

**Scope of Work:**

It is proposed to continue studies of radiation effects in ionic crystalline solids in an effort to obtain answers to the following two questions: a) What are the types of defects that can be introduced by ionizing irradiation; and b) By what mechanism or mechanisms are these defects generated? An answer to one of these questions will undoubtedly provide at least a partial answer to the other question. In particular, attempts will be made to establish the nature of defects complimentary defects other than the H center are not detectable by paramagnetic resonance, techniques such as X-ray diffraction, and optical absorption will be used. Some attention will be devoted to the microscopic strain fields associated with point defects produced by irradiation.

Kinetic studies of the rate of defect production as a function of such parameters as temperature, sample perfection and intensity will be made. It is expected that definite limitations can be placed upon the possible mechanisms of defect production by information obtained in this manner.

The interaction of dislocations with the products of ionizing radiation will also be investigated.

**Contract:** Carnegie Institute of Technology, Pittsburgh,  
Pennsylvania

**Contract Number:** AT(30-1)-3338

**Present Contract Term:** January 1, 1964 through December 31, 1964

**Cost to AEC:** \$26,000

**Contract Title:** APPLICATION OF THE MOSSBAUER EFFECT TO THE STUDY OF  
METALLIC SOLID SOLUTIONS

**Investigators:** Paul A. Flinn

**Scope of Work:**

The Mossbauer effect provides a new technique for investigating metallic solid solutions.  $\text{Fe}^{57}$  and  $\text{Sn}^{119}$  are particularly suitable isotopes for this work, since the effect is relatively large and easily observed, and the elements are of great metallurgical importance.  $\text{Fe}^{57}$  will be used to study the nature and tempering of iron-carbon and iron-nitrogen martensite, particularly the early stages of tempering. Preliminary experiments have shown that changes occur in the Mossbauer pattern before the x-ray diffraction pattern changes. The isomeric shift of the  $\text{Sn}^{119}$  resonance will be measured as a function of electron concentration in Cu-Sn and related alloys, in the hope of gaining a better understanding of the changes of electronic structure with composition in this class of alloys. Since these measurements must be made with great precision to be useful, we are developing an improved type of Mossbauer spectrometer, using a constant velocity electromagnetic drive system.

Contractor: Case Institute of Technology, Cleveland, Ohio

Contract Number: AT(11-1)-588

Present Contract Term: November 1, 1963 through October 31, 1963

Cost to AEC: \$24,915

Contract Title: KINETICS OF PHASE TRANSFORMATION IN ZIRCONIUM-NIOBIUM ALLOYS

Investigators: R. F. Hehemann

Scope of Work:

The transformation of beta to the metastable phase, omega, can take place in a diffusionless manner on quenching or with composition change on isothermal transformation. The athermal reaction takes place reversibly over a broad temperature range. Electrical resistivity and acoustic techniques are being used to study this reversibility of the athermal transformation and the kinetics of the isothermal transformation. Reversion and retrogression constitute important characteristics of the isothermal reaction. Stepped transformation experiments using electrical resistivity and possibly also acoustic techniques will be used to explore these reversion phenomena and their connection with reversibility of the athermal transformation.

Solute segregation in the parent beta phase appears to play an essential role as a pre-transition stage in the isothermal formation of omega. X-ray diffraction has been found to segregate by two different mechanisms. Segregation occurs by a cellular mechanism above and somewhat below the monotectoid temperature. However, decomposition occurs by a different mechanism at lower temperatures. Tentatively, it appears that the low temperature segregation is accomplished by spinodal decomposition. Single crystal and powder diffraction techniques are being used to study this low temperature segregation process and its connection with the omega reaction in a series of zirconium base alloys.

Contractor: Case Institute of Technology, Cleveland, Ohio

Contract Number: AT(11-1)-623

Present Contract Term: February 1, 1964 through January 31, 1965

Cost to AEC: \$80,000

Contract Title: SOLID STATE PHYSICS

Investigators: C. S. Smith

Scope of Work:

Experimental work in thin film physics deals with the magnetic, electrical, mechanical and crystallographic properties of metal films prepared in a modern ultra high vacuum system. It is directed to a basic understanding of these properties and their dependence on preparation variables.

Experimental work on cohesive properties of solids concerns the elastic constant and thermal expansion of single crystals and the pressure and temperature dependence of these properties. The aim is to understand the equation of state and the statistical mechanics of the simple crystals, NaF, LiF, KBr, KI, MgO, and Pb.

The projects in theoretical solid state physics are concerned with the statistical mechanics of idealized condensed systems (3) with the electronic structure of tellurium and of liquids, with the scattering of optical phonons in polar crystals, and with the properties of electrons in magnetic fields.

Recent Publications:

K. H. Rosette and R. W. Hoffman, "Temperature Dependence of Magnetization in Thin Nickel Films," Electrical and Magnetic Properties of Thin Metallic Layers, Koninklijke Vlaamse Academie voor Wetenschappen, Brussels (1962) p. 218.

C. S. Smith and W. B. Daniels, "Pressure Variation of Elastic Constants of Crystals," Physics and Chemistry of High Pressures, Soc. of Chem. Indust., London (1963) p.p. 50-63.

M. J. Klein, "The Onsager Conference," Physisc Today, 16, (1963) p. 145.

M. J. Klein, "Ehrenfest Comes to Leiden: Fifty Years After" Delta 5, (1962) p. 5.

Recent Publications: continued

M. J. Klein, "Planck, Entropy and Quanta, 1901-1906," Natural Philosopher 1, (1963)

R. L. Peterson, "Weak-Coupling Rate Equations and Initial Conditions," Phys. Rev. 130, (1963) p. 612.

H. N. Spector, "Mapping of the Fermi Surface by Means of Magneto-Acoustic Resonances in the Amplification of Sound," Phys. Rev. Letters, 5, (1963) p. 24.

H. N. Spector, "Ultrasonic Amplification in Extrinsic Semiconductors," Phys. Rev., 130, (1963) p. 910.

**Contractor:** The Catholic University of America, Washington, D. C.

**Contract Number:** AT(40-1)-2861

**Present Contract Term:** September 1, 1963 through August 31, 1964

**Cost to AEC:** \$65,764

**Contract Title:** ULTRASONIC STUDIES OF ALKALI METALS

**Investigators:** Paul H. E. Meijer

**Scope of Work:**

An investigation of the Fermi Surface in the alkali metals is being made by the magneto acoustic technique.

Work has included growth of single crystals of potassium and rubidium and preliminary measurements in potassium.

Theoretical work is being done in the fields of paramagnetic resonance and an electron paramagnetic resonance Spectrometer is being built. High frequency ultrasonic measurements are being made in  $Al_2O_3$ .

**Contract:** Chicago, University of, Chicago, Illinois

**Contract Number:** AT(11-1)-357

**Present Contract Term:** January 1, 1964 through December 31, 1964

**Cost to AEC:** \$25,000

**Contract Title:** RESEARCH ON THE SCIENCE OF MATERIALS

**Investigators:** Stuart A. Rice

**Scope of Work:**

This proposal provides partial support of the research of the Institute for the Study of Metals in the form of a one-year contract without detailed specification. The research includes the following subjects of current active interest: Precise determination of crystal structure parameters by X-ray diffraction and neutron diffraction; theoretical and experieental studies on the solid state including metals, semimetals, semiconductors, organic and inorganic crystals and polymers; the experimental techniques include spectroscopy in the visible, ultraviolet, vacuum ultraviolet, infrared and far infrared regions, ultrasonic absorption, microwave absorption, cyclotron and magnetic resonance, thermal, electrical and magnetic measurements, etc. A large number of these experiments will be carried out at very low temperatures. Studies of the transport of matter, energy and momentum, including self-diffusion in solids and liquids, thermal conductivity and viscosity of simple dense liquids; studies of the electronic states of amorphous systems, including liquid metals, metals in molten salts, electrons in simple dense fluids; studies of the thermodynamics of liquid alloys and molten salt mixtures; studies of superconductivity in whiskers and thin films and of the theory of superconducting tunneling, electron-electron superconductivity and related questions; studies of antiferromagnetism; studies of impurity conduction in semiconductors; studies of the optical properties of metals; studies of the Fermi surface of metals and semimetals; studies of magnetic breakdown and the de Haas-van Alphen effect; studies on hydrodynamics and magneto-hydrodynamics of normal fluids and superfluid helium; studies of optical properties of matter in pulsed magnetic fields (500,000 gauss), of crystal fields and of magnetic-lattice relaxation phenomena, of exciton spectra and related topics. Work is in progress to construct an ultra-low temperature and very high magnetic field facility with twelve stations.

**Contract:** Chicago, University of, Chicago, Illinois

**Contract Number:** AT(11-1)-1383

**Present Contract Term:** May 1, 1964 through April 30, 1965

**Cost to AEC:** \$41,301

**Contract Title:** INTERACTIONS ON METALLIC SURFACES

**Investigators:** Robert Gomer

**Scope of Work:**

It is hoped to carry out the following program, largely with the use of field emission techniques:

(1) Adsorption of alkali metals on tungsten and platinum. It is hoped to study adsorption, desorption and surface diffusion quantitatively. After current work on potassium adsorption on tungsten is completed, it is hoped to investigate the adsorption of lithium on tungsten and later on platinum.

(2) Field desorption of lithium. It is hoped to study the desorption of Li from tungsten or platinum under the influence of high electric fields, with a view to learning whether Li adsorption is ionic, and to what extent the interaction of Li<sup>+</sup> ion with a metal surface can be represented by a classic image potential.

(3) Coadsorption. It is hoped to investigate the simultaneous adsorption of various substances on the same substrate to learn whether the same sites are used by both, whether there is competition for these, and whether the more tightly bound adsorbate can displace the weaker one.

Contractor: Cincinnati, University of, Cincinnati, Ohio

Contract Number: AT(11-1)-1115

Present Contract Term: December 1, 1963 through November 30, 1964

Cost to AEC: \$12,490

Contract Title: MECHANISM OF COUNTERDIFFUSION IN METALLIC SYSTEMS

Investigators: Michael Hoch and Frank R. Meeks

**Scope of Work:**

To check closely what is happening and to obtain the various interaction coefficients, the following experiments are carried out: (a) determination of the phase relationships in the copper-rich corner of the aluminum-arsenic-copper system; (b) simultaneous diffusion experiments on four systems: (1) sample of copper containing approximately 8 atomic percent aluminum bonded through a planar interface to a block of copper; (2) sample of copper containing about 2 atomic percent arsenic bonded through a planar interface block of copper; (3) sample of copper containing 8 atomic percent aluminum and a sample of copper containing 2 atomic percent arsenic connected to opposite sides of a block of copper (which is the same configuration as in the published paper; and (4) sample of copper containing 5 atomic percent aluminum and 5 atomic percent arsenic bonded through a planar interface to a block of copper. Configuration 1 gives the diffusion coefficient of aluminum in copper; configuration 2, the diffusion coefficient of arsenic in copper; configuration 3, the counterdiffusion of aluminum and arsenic in copper, and thus the effect that arsenic has on the diffusion coefficient of aluminum in copper and vice versa; and configuration 4, also, the effect which aluminum has on the diffusion coefficient of arsenic in copper and vice versa.

The simultaneous heating and handling of the samples is quite important to eliminate any errors due to small temperature fluctuations and time variations in the diffusion experiments.

**Contract:** Clemson College, Clemson, South Carolina

**Contract Number:** AT(40-1)-3098

**Present Contract Term:** June 1, 1963 through August 31, 1964

**Cost to AEC:** \$66,917

**Contract Title:** RADIATION EFFECTS IN CRYSTALLINE MATERIALS

**Investigators:** R. L. Chaplin

**Scope of Work:**

The primary objective of this research is the study of electron irradiation of metals at temperature near 5°K. The bombarding energy of the electrons is controlled between 0.1 and 0.4 Mev by means of a Van de Graaff accelerator. Currently under study are high purity aluminum and high purity magnesium specimens. Measurements will determine (1) the rate of damage production at different irradiation energies, (2) the recovery behavior of the induced damage, and (3) the relation between physical properties and defects in solids.

**Contract:** Columbia University, New York 27,  
New York

**Contract Number:** AT(30-1)-2921

**Present Contract Term:** February 1, 1964 through January 31, 1965

**Cost to AEC:** \$22,655

**Contract Title:** SHORT CIRCUIT DIFFUSIVITY

**Investigators:** Eugene S. Machlin

**Scope of Work:**

Measurements will be made of the short-circuit conductivity of specific dopants along 100 twist boundaries in KCl as a function of temperature (to obtain activation energy), pressure (to obtain activation volume), misorientation of bounding crystals, size misfit between dopant and potassium ions and excess valence of dopant ions. Also, the feasibility of a technique for purification of alkali halides involving short-circuit enhanced electrolysis parallel to moving grain boundaries will be evaluated. The latter technique will involve several schemes for inducing boundary migration utilizing strain energy as the driving force and for controlling the migration rate by a close control of temperature. The purity of the final product will be evaluated spectroscopically and by measurement of the break temperature between extrinsic and intrinsic conduction.

**Recent Publications:**

D. Jeannotte and E.S. Machlin, "Quenching-in and Annealing-out of Point Defects in Degassed Gold held in Clean and Dirty Atmospheres," Philosophical Magazine, Vol. 8, No. 95 (1963) p. 1835.

Contractor: Connecticut, University of, Storrs, Connecticut  
Contract Number: AT(30-1)-2047  
Present Contract Term: April 15, 1964 through April 14, 1965  
Cost to AEC: \$45,700  
Contract Title: INVESTIGATIONS OF RADIATION EFFECTS IN METAL OXIDES AND METAL AZIDES BY ELECTRON SPIN RESONANCE  
Investigators: Otis R. Gilliam

Scope of Work:

Radiation-induced defects in single crystals of metal oxides and metal azides are being investigated by electron-spin resonance. The radiation is supplied by an electron accelerator, the Brookhaven reactor, gamma-ray sources, and ultraviolet lamps. The major objectives of the research are identification of radiation-induced defects, study of their growth and stability, and correlation of these defects with changes in the properties of the irradiated solids. The major emphasis has been on  $\alpha$ - $\text{Al}_2\text{O}_3$ . The ESR spectra of gamma-ray-irradiated  $\text{Al}_2\text{O}_3$  are attributed to F-centers and to holes trapped at charge-deficient cation sites. Reactor-irradiated  $\text{Al}_2\text{O}_3$  has two prominent ESR spectra; one is attributed to  $(\text{Al O})^{3-}$  molecules formed by replacement collisions, and the other remains unidentified but appears to be a superposition of many spectra. Reactor plus low-temperature gamma irradiation yields a spectrum attributed to interstitial  $\text{O}^\bullet$ . Additional ESR centers specific to electron irradiation have been studied and models are being tested. Observations of interstitial  $\text{O}^\bullet$  establish that the threshold electron energy for oxygen displacements is below 1 Mev. From theoretical investigations of possible defects in  $\text{Al}_2\text{O}_3$ , it has been concluded that  $\text{O}^\bullet$  should have no ESR spectrum at  $0.3 \text{ cm}^{-1}$ , that interstitial  $\text{O}^\bullet$  should have no optical spectrum, and that the defects at cation sites which trap holes are vacancies rather than impurities. In addition, a 7.4-ev optical band has been associated with F centers, a 3.08-ev band with trapped holes, and a 2.00-ev band with interstitial  $\text{O}^\bullet$ . Further measurements will be made with improved resolution, using K-band ESR and ENDOR techniques. Growth, annealing, and threshold energy measurements for production of electron-induced defects in  $\text{Al}_2\text{O}_3$  will continue, and identification of centers will be attempted. Theoretical calculations will be refined and extended to more centers including those induced by electron irradiation. Some effort will be devoted to other materials besides  $\text{Al}_2\text{O}_3$ .

Recent Publications:

F. B. Otto and O. R. Gilliam, "Cryogenic Level Detector and Level Control Circuit," Cryogenics 3, (1963) p.111.

**Contract:** Cornell University, Ithaca, New York

**Contract Number:** AT(30-1)-2150

**Present Contract Term:** April 1, 1964 through March 31, 1965

**Cost to AEC:** \$105,289

**Contract Title:** SOLID STATE PHYSICS: MAGNETIC PHENOMENA

**Investigators:** R. H. Silsbee  
R. Bowers

**Scope of Work:**

The resonance activities under this contract are to be concerned primarily with defects in the alkali halides. These involve the identification of the mechanism responsible for the thermally activated spin lattice relaxation of the F-center in KCl at high temperature and an intensive investigation of the recently discovered R-center resonance which will be carried on in conjunction with optical studies of the same center. Also under study is an F-like center in sodium azide, using ENDOR, and the colloidal sodium resonance in this same material.

The second part of the contract concerns the excitation of magnetoplasma waves in metals and semiconductors. Typical projects include: 1) Studies of wave propagation at very small wavelength where information concerning the Fermi surface can be extracted. 2) Studies in superconductors. 3) Development of fluxmeter for high field measurements based on the magneto-plasma resonance. 4) Studies in Bi and PbTe. 5) Study of surface losses of magneto-plasma waves.

**Recent Publications:**

J. R. Merrill, M. T. Taylor, and J. M. Goodman, "Mode Structure of Standing Helicon Waves in Parallelepiped Samples," Phys. Rev. **131**, (1963) p. 2499

M. T. Taylor and J. M. Merrill, "Doppler Shifted Cyclotron Absorption," Physics Ltrs. **6**, (1963) p. 159

Contract: Cornell University, Ithaca, New York

Contract Number: AT(30-1)-2391

Present Contract Term: April 1, 1964 through March 31, 1965

Cost to AEC: \$182,658

Contract Title: PHONON PHYSICS AND RELATED STUDIES

Investigators: J. A. Krumhansl

Scope of Work:

Scope I is an experimental study of the interactions between phonons and defects using thermal conductivity as the main investigative tool. However, optical and heat capacity techniques are also used. The research is carried out mainly on alkali halides with varying degrees and types of doping. Examples of studies under this scope are: influence of plastic deformation on thermal conductivity; penetration of water into crystals when deformed; alkali halide purification; specific heats at low temperature; thermal conductivity isotope effect, to name a few.

Scope II is a theoretical program concerned with transport properties of solids--mainly thermal conductivity. Examples of studies under this scope are: resonance scattering of phonons by donor electrons in Ge; phonon transport theory in terms of phase states; decay of phonon excitation; second sound in solids; to name a few.

Recent Publications:

R. O. Pohl, "The Applicability of the Debye Model to Thermal Conductivity," Z. Physik, (1963)

C. T. Walker, "Thermal Conductivity of Some Alkali Halides Containing F-Centers," Phys. Rev. 132, (1963) p. 1963.

R. O. Pohl and C. T. Walker, "Phonon Scattering by Point Defects," Phys. Rev. 131, (1963) p. 1433.

A. Griffin and P. Carruthers, "Resonance Fluorescence Scattering of Phonons by Donors and Electrons in Ge," Phys. Rev. 131, (1963) p. 1976.

R. E. Nettleton, "Foundations of Callaway Theory of Thermal Conductivity," Phys. Rev. 132, (1963) p. 2032.

Recent Publications: continued

J. A. Krumhansl, "The Scattering of Lattice Vibrations by Vacancy Type Defects," J. Phys. Chem. Solids, Proceedings of the International Conference on Lattice Dynamics.

A. J. Sievers, III, and M. Tinkham, "Far Infrared Antiferromagnetic Resonance in MnO and NiO," Phys. Rev. 129, (1963) p. 1566; "Far Infrared Spectrum in Fe," ibid. 129, (1963) p. 1995.

Contractor: Cornell University, Ithaca, New York

Contract Number: AT(30-1)-2471

Present Contract Term: October 1, 1963 through September 30, 1964

Cost to AEC: \$57,000

Contract Title: STUDY OF IMPERFECTIONS IN CRYSTALS BY MEANS OF INTERNAL FRICTION MEASUREMENTS

Investigators: H. S. Sack

Scope of Work:

1. The Bordoni peaks of internal friction in Mg and Al are investigated in single crystals with well defined crystallographic orientation and direction of plastic deformation. This permits discrimination between the contributions of dislocations in different slip systems. Further discrimination is obtained by observing the effects of plastic deformation at low and at room temperature of annealing and of point imperfections (impurities and radiation induced defects). The emphasis is on small deformation and on correlation with dislocation structure as observed by thin film electron-microscopy. It is hoped that such systematic work will finally lead to a valid theoretical interpretation.
2. Similar experiments are being made on ionic crystals. Marked differences seem to exist in the effects of point imperfections, the freezing-in of dislocation at low temperatures, etc. One of the experimental difficulties consists in obtaining uniform deformation.
3. The mobility of small angle grain boundaries is studied by means of internal friction. Al with subgrains in different stages of development (produced by the Lacombe method) is studied; the dislocation structure is quantitatively determined by Berg-Barrett X-ray pictures.
4. The dielectric properties of alkali-halides at high temperature were determined earlier at 24 kmc and interpreted in terms of ion vacancy pairs. In order to confirm these results and obtain better estimates for the activation energies of orientation and of dissociation of the pairs these measurements are repeated at 10 kmc. Also the temperature coefficient of the dielectric constant is redetermined with a better precision.
5. The study of electron mobility and lifetime in AgCl by pulsed x-ray irradiation is pushed to lower temperature. Recombination can be distinguished from trapping by simultaneous observation of luminescence.

Recent Publications:

H. S. Sack and G. C. Smith, "Dielectric Properties at High Frequencies and High Temperatures and Point Defect Interaction," Proc. Int. Conf. Crystal Lattice Defects, J. Phys. Soc. Japan 18, Suppl. III, (1963)  
p. 124

**Contract:** Cornell University, Ithaca, New York

**Contract Number:** AT(30-1)-2504

**Present Contract Term:** February 1, 1964 through January 31, 1965

**Cost to AEC:** \$48,410.

**Contract Title:** A STUDY OF RATE CONTROLLING PROCESSES IN DEFORMATION

**Investigators:** Arthur L. Ruoff

**Scope of Work:**

During the past year in the theoretical part of this contract a program has been written and preliminary calculations have been made on the energy of formation of point defects in the alkali metals; a method of accounting for the electron redistribution around a point defect has been used with reasonable success. It is proposed to continue this work during the next year. A detailed analysis of the lifetime of a vacancy in a dislocated crystal has been made. The problem of diffusion from a thick tracer plate into a specimen with concurrent deformation was studied; results on diffusion in nickel under these circumstances were analyzed and shown to give no enhanced diffusion during creep deformation at 0.55  $T_m$ . An analysis was made of space charge effects in creep in ionic crystals.

During the past year in the experimental part of this contract a new creep measuring system has been constructed for continued studies of the effect of temperature and hydrostatic pressure on the alkali metals. This work will be continued. The activation energy and activation volume for high temperature creep in bismuth have been measured. Similar work on single crystal aluminum is now underway. A gas high pressure system has been constructed for use for creep and other measurements at high pressures and temperatures. One of its first uses will be for the measurement of the pressure dependence of diffusion in aluminum by NMR techniques. In the forthcoming year it will also be used in part of the study of the third-order elastic constants in alkali metals.

Contract: Cornell University, Ithaca, New York

Contract Number: AT(30-1)-2558

Present Contract Term: April 15, 1964 through September 14, 1964

Cost to AEC: \$7,905

Contract Title: SOLIDIFICATION REACTIONS

Investigators: H. W. Weart

Scope of Work:

Understanding, and hence control, of eutectic structure and resulting properties is being sought in this study of the details of the redistribution of major components and third elements during eutectic solidification.

A theoretical analysis of steady-state polyphase transformations was made using the thermodynamics of irreversible processes. The predicted relation between interlamellar spacing,  $s$ , and growth velocity  $v$ , viz:  $sv^{1/2} = \text{constant}^*$ , has been quantitatively verified in the Cd-Sn and Sn-Zn systems under this contract and in several other systems by other investigators. Predicted relations between spacing and undercooling for eutectoids cannot be adequately tested for lack of experimental data.

It has been established that, except in unusual circumstances not fully understood, there is no segregation of major components during eutectic solidification, implying that the cellular structure sometimes observed on the solid-liquid eutectic interface is due to impurities. Impurities do segregate, but not as predicted by a simple model. For example, Tl is expected to have an effective distribution coefficient  $k_E$ , in Cd-Sn eutectic of no more than 0.1, but actually has  $k = 0.4$ , as measured by a radioisotope technique.

Projected work for the contract period consists of a more thorough analysis of  $k_E$  including the effect of interface topography; collection of additional data, especially on the effect of growth velocity, on  $k_E$ ; and an attempt to locate the impurity element in the eutectic structure by micro-autoradiography.

\*The relation,  $sv = \text{constant}$ , reported earlier, was found to be incorrect.

**Contract:** Cornell University, Ithaca, New York

**Contract Number:** AT(30-1)-3029

**Present Contract Term:** June 1, 1964 through May 31, 1965

**Cost to AEC:** \$85,602

**Contract Title:** HARD SUPERCONDUCTING MATERIALS

**Investigators:** J. Silcox  
W. W. Webb

**Scope of Work:**

The objective of this work is to determine the effects of defects in the crystal structure of materials such as Nb-25% Zr. and Nb<sub>3</sub>Sn on the magnetic and electrical properties in the superconducting state. Considerable improvement of the current carrying capacity can occur by suitable control of the defect structure but as yet this control is imperfect due to imperfect understanding of the mechanisms. Simultaneous measurements of the D.C. magnetic moment and the electrical resistance transition have been carried out and in conjunction with current theories, these results have been shown to be internally consistent and to give a clearer view of the effects of defects. This work, and parallel theoretical work, will be continued. Measurements of A.C. susceptibility as a function of an applied D.C. bias field are under way on Nb and will be extended to other materials. These measurements supplement the D.C. observations. Work on producing materials with controlled densities of defects is also under way and use will be made of electron microscopy and X-ray diffraction topography for the study of defects in these crystals. In conjunction with this aspect of the program, a liquid helium temperature object stage is being used in the electron microscope for the study of the superconducting transition.

**Recent Publications:**

J. Silcox and R. W. Rollins, "Hysteresis in Hard Superconductors," Applied Phys. Ltrs. Vol. 2, No. 12, (1963) pp. 231-233.

W. W. Webb, "Dislocations in Superconductors," Phys. Review Ltrs., Vol. 11, No. 5, (1963) pp. 191-193.

Contractor: Cornell University, Ithaca, New York

Contract Number: AT(30-1)-3087

Present Contract Term: September 1, 1963 through August 31, 1964

Cost to AEC: \$34,102

Contract Title: CORRELATION OF PHYSICAL PROPERTIES OF CRYSTALS WITH MICROSTRUCTURE

Investigators: John Silcox

**Scope of Work:**

The first year has been spent mainly in the construction of apparatus and the development of techniques. Effort has been spent largely on one problem-- that of the correlation of coercivity with dislocation density in single crystals of nickel. The vibrating magnetometer has been developed for cutting and shaping magnetometer specimens from single crystal tensile specimens and transmission electron microscopy is beginning. Initial results suggest that the apparatus is working satisfactorily and the coercive force has been observed to change from 0.2 to over 30 oe with increasing deformation in line with other observations. Preliminary experiments have also been initiated on quenched and neutron irradiated nickel. Experiments on fatigued or cyclically stressed nickel specimens and observations on domain structure by Bitter pattern and Lorentz microscopy techniques have been initiated.

Contract: Cornell University, Ithaca, New York

Contract Number: AT(30-1)-3228

Present Contract Term: June 7, 1964 through February 6, 1965

Cost to AEC: \$20,700

Contract Title: SOLID LIQUID INTERFACE

Investigators: Che-Yu Li

Scope of Work:

The purpose of this project is to study the structure and the thermodynamics of Solid-Liquid interfaces.

From kinetic data of morphological changes governed by capillarity on interfaces between a solid electrolyte and a liquid electrolyte and between a solid metal and a liquid metal, the interfacial tensions are calculated. The electrical conductivities of a thin film solid electrolyte in contact with liquid electrolytes of different compositions are measured to reveal the defect structure in the solid near the interface.

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PUBLICATION REFERENCE

NOTICE OF RESEARCH PROJECT  
SCIENCE INFORMATION EXCHANGE

SMITHSONIAN INSTITUTION

Atomic Energy Commission  
Division of Research

SIE NO.

AGENCY NO.

REPORTING AGENCY:

TITLE OF PROJECT:

Electronic Properties of Defects in Ionic Crystals

Give names, departments, and official titles of PRINCIPAL INVESTIGATORS and ALL OTHER PROFESSIONAL PERSONNEL engaged on the project.

D. B. Fitchen, Asst. Professor, Physics Department  
Two Graduate Research Assistants

NAME AND ADDRESS OF INSTITUTION:

Physics Department  
Cornell University  
Ithaca, New York

26,680

SUMMARY OF PROPOSED WORK - (200 words or less.) - In the Science Information Exchange summaries of work in progress are exchanged with government and private agencies supporting research, and are forwarded to investigators who request such information. Your summary is to be used for these purposes.

We propose to begin an experimental study of the electronic properties and electron-lattice interaction of certain color centers in alkali halides. The centers selected are those where new features in the optical spectra provide a direct test of the theories of vibrational coupling of color centers. Experiments proposed are (1) an intensive study, through optical absorption and emission spectra, of the temperature and pressure dependence of the intensity, width, and position of zero-phonon lines and the spacing and intensity of vibrational structure for the R, N and other centers, particularly in LiF, for detailed comparison with the theory, (2) a study of the fine structure of the F-center absorption in the cesium halides, particularly in CsF where the splitting is most pronounced and the multiplicity is greatest, and (3) a study of excited state lifetimes of some of these centers, particularly as affected by static and dynamic strains. In this connection, we are equipped for optical studies at hydrostatic pressures up to 10,000 atm at low temperatures, and will also use a simple uniaxial stress device.

SIGNATURE OF  
PRINCIPAL INVESTIGATOR

PROFESSIONAL SCHOOL  
(medical, graduate, etc.)

Lab of Atomic and Solid State Physics  
Cornell University

NOVEMBER, 1964

Paul W. McDaniel, Director  
Division of Research

December 3, 1964

Mark C. Wittels, Metallurgy and Materials  
Programs, Division of Research

**NEW CONTRACT WITH CORNELL UNIVERSITY (BALLUFFI)**

A new proposal entitled "Defects in Metal Crystals" with Professor R. W. Balluffi as principal investigator, has been received and subjected to review. The investigation is essentially an experimental study in two major areas of the crystal (metal) defect field: (1) Interstitial point defect properties, and (2) Sources and sinks for vacancies.

In the first area work is already underway in bombarding oriented metal crystals along channeling directions with metal ions of the same type as the target. By this technique a large concentration of interstitials is produced under controlled temperature conditions, and these will first be observed through transmission electron microscopy and then by electrical resistance measurements. A 20 keV heavy ion accelerator for this work is already in operation and equipment funds this year are requested to upgrade it into a more versatile accelerator. An Hs-11A Hitachi electron microscope including extensive accessories is also available for this research.

Professor Balluffi proposes to initiate these studies with oriented gold single crystals to first establish some of the basic properties of channeled interstitials, including annealing kinetics, defect defocusing at crystal imperfections, debris decoration, and vacancy tetrahedra annihilation. Once a clear insight is gained with the fcc element gold it is planned to extend the studies to other fcc metals, bcc metals, and some selected dilute alloys.

The experimental and theoretical studies of interstitials, to date, have been far from satisfactory and have generally yielded ambiguous results. Since this area is important to a more complete understanding of radiation damage processes a concerted effort, as described in this proposal, is to be welcomed. The recent discovery of pure interstitial production resulting from a high energy channeling phenomenon should offer a good springboard for this attack.

In the second portion of this proposal a study of sources and sinks for vacancies is offered as an important area of research. Again, transmission electron microscopy would be heavily relied upon for the direct observation

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of source and sink action but it is anticipated that other direct methods such as X-ray topography studies would also be employed. The technique would involve rapid high temperature pulse methods to introduce vacancies in fairly perfect crystals so that the obscuring effects of large concentrations of dislocations and sub-boundaries are avoided. An intensive effort would be given to the determination of the spatial distribution of vacancies and the denuded zones around possible sinks in quantitative experiments.

In what might be considered a more applied aspect of this research, study would be given to action at grain boundaries of a controlled nature, and possibly even prepared bicrystals. Several other experiments are also carefully described which involve dislocation climb, loops, jogs, and diffusion pipes, all of which are important to the mechanical properties of metals. The main effort in this part of the proposal is centered upon vacancy phenomena, however.

An original proposal relating only to the interstitial aspects of the research was submitted on September 29, 1964. Shortly thereafter I visited Cornell to attend the MSC information meeting and had the opportunity to discuss the proposal with Professor Balluffi at some length. It developed that he was planning to submit a proposal on the vacancy aspects to another federal agency. I discouraged him from taking this step not only because of the apparent excellence of both areas of study and their significance to our program, but also because of his outstanding record in the field, and to a somewhat lesser degree, because of the undesirability of multiple support. To our mutual benefit, Professor Balluffi agreed to submit one proposal, including both areas of research, to the AEC for review.

This unified proposal has received highly favorable reviews from Vineyard (BNL), Huntington (RPI), and Sosin (AE). As indicated previously the research is important to AEC interests and support is unhesitatingly recommended. The revised budget and funding level shown below appears satisfactory. This revised budget has been requested.

AEC funds	\$147,665 (includes \$79,800 for
Cornell funds	14,487 equipment)
Total	\$162,152

On page 30 of the proposal it is noted that some progress has already been made under ARPA support and this funding will be gradually phased out after AEC support is obtained. Professor Balluffi neither receives nor plans any other agency support at this time.

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Paul W. McDaniel

December 3, 1964

Title to the equipment should be vested in the university since in the event of contract termination it can reasonably be expected that the equipment will continue to be used in research of interest to the AEC.

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**Contract:** Cornell University, Ithaca, New York

**Contract Number:** AT(30-1)-3326

**Present Contract Term:** December 1, 1963 through November 30, 1965

**Cost to AEC:** \$27,670

**Contract Title:** THE THEORY OF SLOW NEUTRON INELASTIC SCATTERING BY LIQUIDS

**Investigators:** Mark Nelkin

**Scope of Work:**

The time dependent position correlations for some dynamical models of classical fluids will be calculated. It is hoped to thus develop an improved physical understanding of the dynamical mechanisms determining the inelastic scattering of slow neutrons by liquids. Given a formally well developed theory, such insight is best obtained from judiciously chosen model calculations. The primary emphasis in the research will be on a binary collision model as applied to a hard sphere fluid. At low densities, old and new existing calculations from the Boltzmann equation will be extended. At higher densities, the method of calculation has not yet been decided. It is planned to maintain close contact with the current literature on the molecular theory of liquids, and to correlate the model calculations of inelastic neutron scattering with those for the equilibrium and transport properties. It is hoped that this will be facilitated by using the formalism of thermodynamic Green's functions.

Calculations will also be carried out for hindered rotations in molecular systems since considerable neutron scattering data exists in this area, and a theory exists which has not been adequately compared with experiment.

**Contract:** Denver, University of, (Colorado Seminary), Denver, Colorado

**Contract Number:** AT(11-1)-1298

**Present Contract Term:** June 1, 1964 through May 31, 1965

**Cost to AEC:** \$26,175

**Contract Title:** ALLOYING BEHAVIOR OF THE RARE EARTHS

**Investigators:** C. E. Lundin

**Scope of Work:**

The overall objectives of this research are to provide a better understanding of alloying behavior using binary intra-rare earth alloys as a basis. The rare earths were selected because of their well-behaved properties. Alloy systems can be selected with fewer property variables, so that their alloying characteristics can be studied under more controlled conditions.

An investigation of the binary system Y-Gd is proposed for the next contract period. The investigation will follow the same pattern as has the previous and present studies on the systems Pr-Nd and Sm-Gd, respectively. The phase diagram of the Y-Gd system will be determined by a combination of metallography, X-ray diffraction analysis, thermal analysis and density measurements. A determination will be made of solution ideality in the solid and liquid solutions by employing the Knudsen effusion apparatus. First the vapor pressures of the pure components will be established. Then various alloy compositions will be studied to determine the vapor pressure of one component in the combined vapors over the liquid and solid solutions. The alloys for this study will be arc melted in compositional increments of 10 atomic percent. Each alloy will be heated in the effusion cell until sufficient condensate is collected on a platinum target. The condensate will be analyzed by X-ray fluorescence techniques to determine the atom fraction of the components in the vapor. Each alloy composition will be evaporated at 3 different temperatures in the liquid solution and 3 different temperatures in the solid solution. Then, based upon the Gibbs-Duhem relation, the activities of one component in solution of both components will be computed. It is also proposed to determine specific volumes throughout the Y-Gd system by precision back reflection X-ray techniques of alloys in the solid state. From these data the atomic volume vs. composition relationship will be plotted to determine whether the system exhibits ideality in the solid state at room temperature.

**Contract:** Emory University, Atlanta, Georgia

**Contract Number:** AT(40-1)-2953

**Present Contract Term:** January 1, 1964 through December 31, 1964

**Cost to AEC:** No-fund Extension

**Contract Title:** THE DETERMINATION OF LOW ENERGY X-RAY ABSORPTION COEFFICIENTS

**Investigators:** Robert H. Rohrer  
Randall W. Carter

**Scope of Work:**

Measurements are being made of X-ray mass absorption coefficients of elements having atomic numbers ranging from about 32 to 12 for x-ray energies from 6 kev to somewhat less than 1 kev. Data taken for the elements Ge, Zn, Cu, and Mn indicate that, for energies less than 3 kev, there is an increasing deviation from mass absorption coefficient values predicted by published empirical equations. The experimental values are higher than the predicted values.

Mass absorption coefficients of additional elements will be measured and the data will be analyzed for trends of deviations from theoretical values as functions of energy and of atomic number in an effort to establish a more reliable functional representation of these values.

**Contract:** Florida, University of, Gainesville, Florida

**Contract Number:** AT(40-1)-2581

**Present Contract Term:** June 1, 1964 through May 31, 1965

**Cost to AEC:** \$40,975

**Contract Title:** TOPOLOGICAL STUDY OF THE SINTERING PROCESS

**Investigators:** Frederick N. Rhines  
John Kronsbein

**Scope of Work:**

The work which is being conducted embodies a continuation of the application of network topology and quantitative metallography to the determination of the evolution of structure during sintering. It is an extension of the study of effects of initial configuration and subsequent environment upon the linear surface area-density relationship which had been established in earlier research at this laboratory. Encompassed by this extension of effort are effects of particle size distribution, material being sintered, and study of the relationship in multi-phase sintering. An additional parameter, which metallographically estimates total length of intervoidal channels in the system, adds further breadth to the investigation.

Concurrently, precision determinations of the kinetics of densification and the sintering force (load required to bring the shrinkage rate to zero) are being carried out, with emphasis upon the effects of the same configurational and environmental variables listed in the first paragraph.

Finally, correlations between various aspects of structure with mechanical properties, notably hardness, fracture strength, and elongation are being continued.

Contract: Florida, University of, Gainesville, Florida

Contract Number: AT(40-1)-3262

Present Contract Term: June 1, 1964 through May 31, 1965

Cost to AEC: \$24,011

Contract Title: DEFORMATION PROCESSES IN ZIRCONIUM

Investigators: R. E. Reed-Hill

Scope of Work:

The objective of this program is to study internal friction phenomena in zirconium prestrained at 77°K so as to nucleate large numbers of twins. The internal friction effects in question are believed to be associated with anelastic movements of twin boundaries. It is hoped that this investigation will lead to a better understanding of the dislocation structure of non-coherent twin boundaries and the mechanisms that control the movements of these dislocations as the twins grow in size.

Four basic techniques of measurement will be employed. These are:

- a. Cyclic stress-strain tests performed on the Instron machine.
- b. Elastic after effect tests.
- c. Constant-stress strain-time curves. In these tests the specimens will be loaded to a fixed stress and the development of the anelastic strain will be measured as a function of the time of application of the stress.
- d. Torsion pendulum tests. The techniques described above are envisioned for specimens to be tested in the vicinity of room temperature. At temperatures of the order of 100°C, however, relaxation occurs in the order of seconds and the use of a torsion pendulum would be more appropriate to the study of the phenomena in this temperature range.

A goal of the research will be to determine the functional relationships between the various dislocation related variables and such other pertinent variables as time, strain and stress.

**Contract:** Franklin Institute Laboratories, Philadelphia,  
Pennsylvania

**Contract Number:** AT(30-1)-2730

**Present Contract Term:** January 15, 1964 through January 14, 1965

**Cost to AEC:** \$25,000

**Contract Title:** SOLID STATE INVESTIGATIONS UTILIZING ELECTRON-BOMBARDMENT  
PHENOMENA

**Investigators:** Martin Pomerantz

**Scope of Work:**

The objective of this project is to achieve understanding of effects produced by bombardment of crystalline solids with electrons. Traversal of solids by high energy electrons gives rise to certain conductivity phenomena, the analysis of which provides information regarding the electronic structure of the material. Bombardment of surfaces may cause removal of surface atoms and observation of these effects yields knowledge of binding energy and surface structure.

Studies of conductivity of magnesium oxide single crystals induced by irradiation with fast electrons are nearing completion. The anomalous result concerning decay of conductivity at low temperatures has been traced to the existence of several impurity levels. Measurements of the thermally-stimulated conductivity following bombardment have helped to identify the trapping levels contributing at different temperatures. A theoretical model has been proposed to account for the time dependence of the decay of conductivity in the case of crystals where only one level contributes and the parameters have been determined by machine calculation. Specific additional topics to be pursued with the MgO are: (1) introduction of known impurities, (2) emptying of trapping centers by optical means and determination of wavelength dependence of this effect if it occurs, (3) observation of thermoelectric effect in MgO to determine nature of the major carrier, and (4) measurements with other wide gap materials (e.g. BeO and SiO<sub>2</sub>) to test the generality of the model.

Means will be investigated for observing displacements and/or removal of surface atoms by particle irradiation. Initial studies will be directed toward effects of electron bombardment upon a thorium monolayer on tungsten, and the study of such effects by low energy electron diffraction. Calculations of displacement cross sections will be carried out for a wide range of mass, incident energy, and energy required for displacement. Extension of the work to include neutron and heavy-particle irradiation is planned.

Recent Publications:

G. L. Sewell, "Model of Thermally Activated Hopping Motion in Solids", Phys. Rev. 129, 597 (1963).

Newton I. Greenberg, "Binary Kernel Formulation of a Heisenberg Model of Ferromagnetism", J. Math. Phys. 4, 405 (1963).

Arvid A. Schultz and Martin A. Pomerantz, "Secondary Electron Emission Produced by Relativistic Primary Electrons", Phys. Rev. 130, 2135 (1963).

**Contract:** The Franklin Institute Laboratories, Philadelphia 3,  
Pennsylvania

**Contract Number:** AT(30-1)-2994

**Present Contract Term:** March 1, 1964 through April 30, 1964

**Cost to AEC:** No-fund Extension

**Contract Title:** STRUCTURE OF VAPOR-DEPOSITED THIN FILMS

**Investigators:** R. W. Vook

**Scope of Work:**

An in-situ x-ray investigation of the structure of high vacuum evaporated metal films is being carried out. The results obtained so far refer to copper films deposited on glass substrates at liquid nitrogen and room temperature. It has been found that the stacking fault density of films deposited at liquid nitrogen temperature varies between .010 and .016 stacking faults/plane. The twin fault density varies between .03 and .10 for (111) oriented grains and between .21 and .43 for (100) oriented grains. All the line broadening in films deposited at the low temperature can be accounted for by the presence of twins and stacking faults. This means that the grain size is greater than 1000 and that the strain in the film is small. The as-deposited film at liquid nitrogen temperature has a moderate (111)-texture. When it is warmed to room temperature, there is a tendency to the formation of a strong (100) texture. Future investigations will be concerned with an electron microscope identification of the defects present in annealed films. The major new effort will continue the quantitative x-ray investigations. We expect to obtain values of the grain size and strain from a Warren-Averbach analysis of diffraction line shapes. Secondly, films will be deposited on NaCl and the results compared to those obtained from films deposited on glass. Finally, a more careful investigation of the annealing processes will be initiated.

**Recent Publications:**

J. Takamura, K. Okazaki and I. G. Greenfield, "Quenched in Vacancies in Dilute Aluminum-Magnesium Alloys," J. Phys. Soc., Japan 18, Supplement III (1963) p. 78

I. G. Greenfield and H. G. F. Wilsdorf, "Point Defect Clustering in Nickel," J. Phys. Soc., Japan 18, Supplement III, (1963) p. 20.

**Contract:** Georgia Institute of Technology, Atlanta, Georgia

**Contract Number:** AT(40-1)-2755

**Present Contract Term:** June 1, 1964 through May 31, 1965

**Cost to AEC:** \$68,160

**Contract Title:** SURFACE PROPERTIES OF MAGNETIC MATERIALS

**Investigators:** Edwin J. Scheibner

**Scope of Work:**

The purpose of the research is to investigate various properties of the surfaces of magnetic materials. During the first four years under this contract, the research included three types of studies. (1) Instrumentation was developed for measuring the magnetic properties of thin nickel films in the thickness range where size effects would be expected to predominate. Studies were then performed on silicon monoxide-overcoated nickel films with a torsion magnetometer and on pure nickel films evaporated and measured in ultra-high vacuum with a sensitive hysteresis loop tracer. Concurrently, theoretical studies were made of the effect of boundaries on the magnetization of thin ferromagnetic films. (2) Studies were made of gas phase-metal surface reactions, particularly the carbon monoxide attack of stainless steels and thin films of iron and nickel. Electron microscopy was used extensively to examine the initial stages of the CO reaction. (3) Low energy electron diffraction (LEED) equipment for investigating surface structures was designed during the past year and theoretical studies are being made on methods for determining the vibrations of surface atoms by the LEED technique.

In the proposed research these studies will be continued with the major effort devoted to the low energy electron diffraction work, the magnetic phenomena observed in thin films near the Curie point, and the elucidation of the mechanism and conditions for growth of filamentary carbon during the gaseous reactions.

**Contractor:** Harvard University, Cambridge, Massachusetts

**Contract Number:** AT(30-1)-1956

**Present Contract Term:** September 1, 1964 through August 31, 1965

**Cost to AEC:** \$16,655

**Contract Title:** REACTIONS BETWEEN SOLID AND LIQUID METALS ALLOYS

**Investigators:** Bruce Chalmers

**Scope of Work:**

The kinetics and morphology of ice growing in water at large amounts of supercooling ( $8^{\circ}$  to  $30^{\circ}$ ) will be studied. The relationship between rate of growth and temperature will provide new information about the growth of an isolated dendritic tip, while the morphology will indicate the extent of interaction between adjacent branches.

The study of the interaction between the solid-liquid interface and solid particles will be extended to metallic systems, to test the validity of predictions that have been made on the basis of our recent work on transparent systems. An attempt will be made to measure directly the force exerted by the interface on the particle.

Further experiments will be made with a view to determining the criteria that govern dynamic nucleation; that is, the nucleation of solid crystals in supercooled liquids at temperatures in which nucleation does not take place in the absence of dynamic effects. In particular, the influence of nucleation catalysts on dynamic nucleation will be studied.

Contractor: Houston, University of, Houston, Texas

Contract Number: AT(40-1)-2573

Present Contract Term: February 1, 1964 through January 31, 1965

Cost to AEC: \$54,918

Contract Title: SPUTTERING BY ION BOMBARDMENT

Investigators: John C. Allred

Scope of Work:

The project is the general study of sputtering of metals by inert gas ion beams in the energy range 10-200 kev. Yields, and distribution of sputtered particles, from both polycrystalline and single crystal targets are being measured, also the dependence of these factors on beam direction is being measured. Velocities and momentum of sputtered particles are being measured. Studies of dislocations produced in single crystals by ion bombardment are also being made. Particular attention in all these measurements is made to sputtering of copper, silver, nickel, and cobalt by Argon ion beams.

Measurement of sputtering is made by collection of sputtered material on glass plates and oscillating quartz crystals, and measuring the thickness of the film on glass by interferometry, or the change in frequency of the quartz crystals.

Experiments are also being performed to determine the effect if any of target temperature on the sputtering parameters of both polycrystalline and single crystal targets.

Current densities are of the order of  $100 \text{ a/cm}^2$  or larger, and vacuum condition  $2 \times 10^{-6} \text{ mm Hg}$  or better.

**Contract:** IIT Research Institute

**Contract Number:** AT(11-1)-578, Project #9

**Present Contract Term:** February 15, 1964 through February 14, 1965

**Cost to AEC:** \$59,966

**Contract Title:** MAGNETIC PROPERTIES OF INSULATORS

**Investigators:** J. J. Markham

**Scope of Work:**

This program involves a continuing investigation into the magnetic and optical properties of point defects in solids. Specifically, the concern is with semi-localized, paramagnetic centers whose electron or electrons spread out into the region occupied by the ions surrounding the center. At present, the investigation is applied to the F-center in alkali halides which is an electron trapped at a negative ion vacancy. The major problem at this time is to understand the interaction of the trapped electron with its environment. One may saturate a fraction of the magnetic resonance absorption line, i.e. burn a hole in it. Measurements of its width and shape as well as its relaxation time at various temperatures and concentrations can lead, by means of the theory, to a determination of the interaction mechanisms between the trapped electron and the lattice. The experimental and theoretical investigation of the electron resonance absorption by this laboratory as well as others have led to a fairly good understanding of the mechanisms which define the total resonance line of the F-center. While there has been considerable research on the partially saturated resonance (the "hole") by this laboratory, its unusual features await a more detailed experimental and theoretical investigation. It is not sufficient, however, to consider only the magnetic lattice vibrations. This can be examined most effectively by means of the optical properties of the system. In addition, it is partly through optical measurements that a "pure" F-center can be defined to ensure that this is the only magnetic center involved in the resonance experiments.

**Recent Publications:**

T. N. Casselman and J. J. Markham, "Some Effects of a Perturbation in a Lattice on the Normal Modes", J. Phys. Chem. Solids 24, (1963) p. 669.

**Contract:** Illinois Institute of Technology, Chicago, Illinois

**Contract Number:** AT(11-1)-1052

**Present Contract Term:** June 15, 1964 through June 14, 1965

**Cost to AEC:** \$29,713

**Contract Title:** INVESTIGATION OF ENERGY TRANSFER PROCESSES BY FLASH PHOTOLYSIS

**Investigators:** Leonard I. Grossweiner

**Scope of Work:**

This program comprises research on aspects of radiation effects in ionic solids. Measurements of the fracture surface energy of KCl show that gamma-ray irradiation causes a significant decrease in the (100) surface energy which is attributed to the introduction of lattice strain. The subsequent changes induced by optical bleaching of the F band and thermal annealing indicates that the coincident increase in hardness and decrease in surface energy are not due to identical defects. Measurements on the related surface property of self-friction show that irradiation causes an increase in the adhesion contribution to friction and a decrease in the ploughing contribution. The analysis with friction theory indicates that the former is controlled by elastic deformations and the latter by plastic flow.

Investigation of rapid color center transformations with pulse-bleaching techniques show that the interconversion of F and F' centers in KCl at low temperature is altered markedly by the presence of aggregate centers. The results indicate that the interactions due to a condensation of F centers which occurs during the earliest stages of optical bleaching differ from those due to coagulation into distinct color center aggregates. Room-temperature pulse bleaching studies show that photo-ionization of M or N centers leads to temporary absorption bands not associated with the known aggregate centers. However, the new bands have been stabilized by simultaneous optical bleaching of the F band with the N or M bands at 100 C and they are attributed to distinct higher aggregates.

The investigation of the sensitization of zinc oxide film photoconductivity by organic dyes shows that p-type eosin sensitizes by hole transfer and capture at zinc oxide recombination centers. The kinetics of the fast electronic processes occurring in the dye film and slower steps in the zinc oxide film have been studied with pulse methods. The current work includes an extension to sensitization by n-type methylene blue.

**Contract:** University of Illinois, Urbana, Illinois

**Contract Number:** AT(11-1)-1046

**Present Contract Term:** June 1, 1964 through May 30, 1965

**Cost to AEC:** \$ 16,000

**Contract Title:** MECHANICAL BEHAVIOR OF DILUTE ALLOYS OF NIOBIUM

**Investigators:** G. M. Sinclair

**Scope of Work:**

The critical resolved shear stress for niobium single crystals having different substructures will be determined at temperatures between 78°K and 450°K and for strain rates between  $10^{-2}$  and  $10^{-6}$  per second. The crystals will be oriented with  $[110]$  parallel to the compression axis. Different substructures will be produced by controlled plastic prestrain and subsequent recovery heat treatment. Etch pitting techniques will be used to define substructure. The data obtained will be employed to examine the effect of substructure on the frequency factor, activation volume and friction stress of the deformation rate equation for this material.

**Recent Publications:**

J. Cost and C.A. Wert, "Metal-Gas Equilibrium in the Niobium-Nitrogen Terminal Solid Solution" Acta Metallurgica, 11:4, April 1963, p. 231.

D. C. Huffaker and G. M. Sinclair, "Yield Behavior of Polycrystalline Niobium," ASME Paper 63-WA-117, November 1963 (To appear in Transactions of ASME - Journal of Basic Engineering)

Contractor: Illinois, University of, Urbana, Illinois

Contract Number: AT(11-1)-1198

Present Contract Term:

Cost to AEC: \$1,581,000

Contract Title: THE SCIENCE OF MATERIALS

Investigators: R. J. Maurer and Associates

Scope of Work:

This master contract is a major support of the Materials Research Laboratory of the University of Illinois. The Advanced Research Projects Agency of the Department of Defense also gives support to the work of the Laboratory, which is an interdepartmental organization of five departments (Ceramics, Chemistry and Chemical Engineering, Electrical Engineering, Metallurgy, and Physics), for the purpose of fundamental research on the properties of solids. This program includes investigations of the mechanical, electrical, magnetic and optical properties of solids. The following projects constitute the part of the program that is supported by the U. S. Atomic Energy Commission.

I. Very Low Temperature Properties of Solids

A. Properties of Rare Gas Solids - R. O. Simmons

This project aims to grow and to study mm to cm size crystals of neon and argon. Specifically, it aims to develop techniques for manipulation of such crystals, to verify directly their crystalline perfection by x-ray diffraction techniques, to measure as a function of temperature their lattice constants, their thermal expansivity, their isothermal compressibility, and the intensities of selected Laue-Bragg diffraction maxima. These data will be compared to measurements of other thermodynamic properties and to existing theories of crystal lattice dynamics.

Particular emphasis will be placed upon the temperature interval between 2 and 30°K and the pressure range below 100 atmospheres, for which very few single crystal data exist. Study of Ne<sup>20</sup> and Ne<sup>22</sup> crystals, in which zero-point effects are present but not predominant, will be used to investigate the influence of zero-point and anharmonic effects.

B. Research on the Properties of Materials at Low Temperatures - J. C. Wheatley

The work will be primarily concerned with the cooling of liquid and solid He<sup>3</sup> to temperatures well below 0.01°K. At such temperatures a search will be made for a highly correlated phase of liquid He<sup>3</sup> which has been predicted from the BCS theory. An attempt will be made to observe the propagation of zero sound as predicted by Landau. An attempt will be made to more accurately determine the limits of validity and the parameters for the Fermi liquid theory as applied to He<sup>3</sup>. The experimental approach is dictated by the present development of refrigeration and thermal isolation techniques. The most likely properties of He<sup>3</sup> to be measured are the diffusion coefficient, the magnetic susceptibility, the thermal diffusivity, the velocity and attenuation of sound. Quantitative measurements will also be made on He<sup>3</sup> at temperatures above 0.01°K that are presently accessible.

II. Intrinsic Structure and Properties of Solids

A. Electronic Specific Heat Study of the Alloys of Transition Elements - P. A. Beck

The electronic specific heat of bcc alloys of 3d transition elements with nontransition elements such as aluminum are being measured as a function of electron concentration. Similar studies are being made with bcc alloys of 4d and 5d transition elements with one another. Low temperature specific heat measurements are being made in a magnetic field with superconductive alloys of the Ti-V system.

Past results indicate that the electronic specific heat of alloys of transition elements with one another can be described in terms of a more or less rigid band; the degree of filling of this band being determined by the average electron concentration of the alloy. Such an explanation of the specific heat data of alloys involving nontransition elements such as Al, Sn, and Sb does not seem possible. The effect of nontransition elements on the shape of the d band is being examined by determining the electronic specific heat of alloys over a relatively wide range of electron concentration with fixed amounts of nontransition element additions.

A study of bcc solid solutions in the systems Zr-Nb, Nb-Mo, and Mo-Re is contemplated. In the Ti-V alloy system, the critical magnetic field versus temperature curve will be measured.

## B. Semiconducting Glasses - W. D. Compton and A. L. Friedberg

Semiconducting glasses of the system  $V_2O_5-P_2O_5$  are to be investigated. Initially, work is to be carried out in the preparation of high purity, homogeneous, crystal-free glasses with as high a vanadia content as possible. Attempts will be made to produce glasses starting with  $V_2O_3$  rather than  $V_2O_5$  and to determine the effect of oxygen pressure during melting on the conductivity of annealed glass specimens.

It is also proposed to measure dc electrical conductivity, thermoelectric power, photoconductivity, and Hall effect in order to gain a better insight on the mechanism of electrical conduction in these glass systems.

Also, with the use of absorption spectroscopy on thin films of glass (blown from the molten glass prior to casting into specimen shapes), it is hoped to learn the concentration of the different cationic species of vanadium that exist in the glasses.

## C. Particulate Glass Systems - A. L. Friedberg

Particulate glass systems have been studied in the past with regard to their usefulness as ceramic coatings and, more recently, as ceramic structures. These systems are formed, mainly, by sintering or coalescence of particles. Investigation of the glass sintering phenomenon has shown that transport of matter takes place chiefly through viscous flow. Grain boundaries in particulate glass systems appear similar in behavior to those of crystalline sintered systems.

The purpose of the program is the study of the sintering phenomenon in particulate glass systems with emphasis on not only the sintering kinetics but also on other characteristics of these systems, such as gas solubility and crystallization behavior, that are associated with the large specific surface.

The initial program, exploratory in nature, will concentrate on (a) the kinetics of grain boundary formation and disappearance, (b) techniques for delineating the interfacial surfaces of grain boundary material and (c) the effect of environment on the sintering kinetics. It is proposed to begin work with lead borate and lead silicate glasses that have been well characterized in this laboratory with respect to certain properties such as viscosity and electrical conductivity.

## D. Use of Very High Pressure to Investigate the Structure of Matter - H. G. Drickamer

The purpose of this project is the investigation of intermolecular and intramolecular forces, using high pressure as a primary tool. At present experimental techniques have been

developed to permit optical absorption studies to 160 kilobars, electrical resistance measurements to 600 kilobars, x-ray scattering measurements to over 500 kilobars, and Mössbauer measurements to perhaps 300 kilobars. Apparatus is currently being developed for NMR studies at high pressure.

Projects currently being undertaken include: (1) optical absorption and electrical resistance measurements on fused ring aromatic compounds and on charge transfer complexes, (2) electrical resistance measurements on transition metals, (3) lattice parameter measurements on simple ionic crystals, e.g., NaCl, CsCl, KCl, MgO, CaO<sub>3</sub>, (4) lattice parameter measurements of the alkali metals, (5) lattice parameter measurements for hexagonal crystals, (6) studies of structure and compressibility of the high pressure phases of Si, Ge, and various compounds having the zinc blende structure, (7) Mössbauer studies on Fe<sup>57</sup> in iron and in titanium, and (8) NMR studies on the high pressure phases of InSb and of cesium.

#### E. Crystal Growth and Surface Properties - J. J. Gilman

The techniques for growth of pure, perfect crystals of refractory, high temperature compounds will be studied. Typical examples of the compounds under consideration are tungsten carbide and silicon carbide. These crystals possess unusual elastic and mechanical properties which are of particular interest from both a practical and theoretical point of view.

A second phase of the program is concerned with the surface properties of crystals, particularly the transition metal compounds, and of polymers. The surface structures will be examined through use of both field ion microscopy and low energy electron diffraction techniques.

#### F. Anharmonic Effects in Solids - A. V. Granato

Anharmonic properties of solids are to be studied using ultrasonic techniques. Data is to be collected on the elastic constants, together with the temperature and stress coefficients of the elastic constants of a wide range of materials. The immediate objectives of the program are the development, collection and testing of equipment, the preparation of specimens and the measurement of the second order elastic constants of some materials in the alkali halide and the noble metal groups. In the case of the alkali halides, theories are fairly well developed and the measurements should serve as a check for the theories. In the case of the noble metals, theoretical work seems to be less firmly based, and the measurements may be useful in guiding further developments.

Longer range objectives of the program are the collection of data accurate enough (1) to be useful in the checking of relations which may exist between various anharmonic effects, (2) to serve as a check and a guide for theories of the solid state, (3) to establish useful equations of state for solids, (4) to determine interatomic potentials, and (5) to calculate defect properties in crystals.

#### G. Nuclear Magnetic Resonance Studies - T. J. Rowland

An investigation of the effects of small quantities of various solute elements on the nuclear magnetic resonance intensity of metallic copper is to be carried out. The concentration range of interest is of the order of 0.1 atomic percent. Zinc is the solute to be used initially. Effects and methods of annealing the samples, which will be filings from bulk material, are very important and will receive extensive study. At these small concentrations first order quadrupole perturbation of the Zeeman levels should be the predominant observable effect.

The studies of the Knight shifts of a number of solute species in copper and silver base solid solutions are being completed.

The high field (30,000 gauss) line shape of dilute (of the order of 0.5 atomic percent) silver alloys is to be examined. This may assist in determining the change in electron density at the near neighboring sites of substitutional solute atoms in these solid solutions.

Apparatus is being constructed to measure relaxation times in metals and alloys. In particular we are interested in applying a technique, recently developed by Slichter, to alloys and intermetallic compounds. It should be possible in some cases to measure the lattice jump time and thus the diffusion rate in these materials. Further studies are being made to determine the applicability of the method to metallurgical problems of interest, such as the activation energy for diffusion and/or vacancy concentration in situations where the vacancy concentration depends on the alloy composition.

#### H. Dielectric and Structural Investigation of Complex Compounds of the Perovskite Type $ABO_3$ - V. J. Tennery

A search for new oxide ferroelectric crystals having the perovskite structure is the primary subject of this investigation. The electrical properties and crystalline symmetry of complex compounds are presently being determined. Work in the Soviet Union and more recently in the United States has demonstrated

that complex compounds such as  $\text{Pb}(\text{Sc}_{0.5}\text{Nb}_{0.5})\text{O}_3$  are single phase perovskites which are ferroelectric below some critical transformation temperature and that they exhibit large spontaneous polarizations while in the ferroelectric state.

This program is initially concerned with establishing if the complex compound  $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3$  is ferroelectric, and to determine its crystalline symmetry and its relative permittivity and dielectric loss as functions of temperature. If ferroelectricity is found in this compound, the system  $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3\text{-PbTiO}_3$  will be investigated to establish the dependence of the ferroelectric properties upon the replacement of  $\text{Ti}^{+4}$  ions by the  $(\text{Zn}_{1/3}^{+2}\text{Nb}_{2/3}^{+5})^{+4}$  group in the known ferroelectric perovskite  $\text{PbTiO}_3$ .

### III. Defect-Controlled Properties of Solids

#### A. Point Defect - Dislocation Interactions - H. K. Birnbaum

The mechanism of point defect formation during plastic deformation of aluminum will be studied using a low temperature strain aging technique. An attempt will be made to determine the nature of these defects and their interactions with dislocations.

The vacancy and divacancy interactions with dislocations will be examined by measuring the internal friction and elastic moduli after quenching gold and aluminum. The kinetics of dislocation pinning and the nature of the pinning points will be studied. An examination of the kinetics of pinning point motion along the dislocation lines will be undertaken.

Measurement of self diffusion along isolated edge and screw dislocations will be continued on nickel and extended to gold. The effect of stacking fault energy and dislocation type on the dislocation self diffusion activation energy will be obtained.

Transmission electron microscope studies of electron bombardment damage in LiF will be continued. The annealing processes after irradiation are being investigated. Studies of the mechanism of formation and nature of dislocation dipoles produced by plastic deformation will be carried out.

#### B. Color Centers in the Alkali Halides - W. D. Compton

The shift in the absorption spectrum of the F center in the presence of an applied electric field is being investigated in an effort to determine the position of the excited 2S state relative to the excited 2p state. Preliminary results on KCl at 110°K and 60°K indicate that the absorption band shifts to higher

energies, and that this magnitude of the shift is proportional to the square of the applied electric field. These measurements are currently being extended to lower temperatures and to other materials. A theoretical analysis of these results is expected to yield, in addition to the relative positions of the 2S and 2p levels, an indication of the local field which the defects experience when an applied field is present.

C. Low Temperature Thermal Conductivity Studies - M. V. Klein

The effect of point defects on the thermal conductivity of alkali halides is our first concern. We have an effective chlorine treatment for removing oxides and related impurities in alkali chlorides and are now growing pure and doped alkali halides for thermal conductivity and optical studies. We want to learn if the very large phonon scattering observed earlier in NaCl-NaOH extends to other similar systems. Caldwell's thesis will be on phonon scattering by monovalent impurities in NaCl.

Equipment is being assembled for high resolution low temperature infrared absorption studies on the hydroxide-doped crystals. Earlier measurements this year at low resolution have revealed some interesting effects that should ultimately tell us much about the dynamics of the Oh ion in the host lattice. We are also setting up to perform Ramon scattering experiments on OH and other defects.

D. Research on Radiation Damage - J. S. Koehler

This project aims to determine the nature and number of lattice imperfections introduced into crystalline solids by nuclear irradiation at liquid helium temperature. In addition, it would like to discover the nature of the various annealing processes which occur as the temperature of the specimen is increased. The activation energy or spectrum of activation energies associated with the motion of each particular lattice defect also constitutes a portion of the desired information. The project also aims to determine the nature and magnitude of the changes in physical properties which result from a given concentration of a particular kind of lattice defect. The defects which are believed to be of importance are interstitial atoms, lattice vacancies, crowdions, small inclusions of another solid phase and possible precipitates of interstitial atoms. The properties investigated will be resistivity, volume, lattice parameter and stored energy. The crystals examined will be copper, silver, gold, iron, nickel, cobalt, GaSb, InSb, germanium, silicon and various alloys.

#### E. Point Defects in Solids - D. Lazarus

The program is concerned with experimental and theoretical studies of the processes surrounding the formation and motion of point defects in solids, with particular emphasis on their role in diffusion. Experimental techniques employed include tracer diffusion studies, nuclear magnetic resonance, internal friction, and microvolt potentiometry. Studies are underway on vacancy-impurity and vacancy-vacancy interactions in noble metals and dilute alloys, on diffusion in refractory metals at high temperatures and high pressures, on the effects of high pressure on the high-temperature electrical resistivity and thermoelectric power of various metals, and on the effects of large electrical currents on mass transport in metals. Some of these involve new apparatus for generation of hydrostatic pressures in gas up to 10,000 atmospheres, and special furnaces to permit long time heat treatment at temperatures exceeding 2000°C.

#### F. Dislocations and Surface Barriers - M. Metzger

A study just completed has shown that the bulk plastic properties of copper crystals are affected by a chromium coating at strains of only 0.01. The nature of interaction between dislocations and the coating and the formation of barriers within the crystal will be investigated by microstrain measurements of flow stress and hysteresis loops and by dislocation etch pit methods.

Current work with specially oriented zinc crystals indicates that copper coatings produce a significant hardening by interaction with screw dislocations but not with edge dislocations. For effective interpretation of these results, it will be necessary to make some observations on the behavior of the coating.

One possible result of the interaction of dislocations and a coating is detachment of the coating. The kinetics of this effect were under study by a photomicrographic method in oriented aluminum single crystals and polycrystals with an oxide film. This study will be completed.

In work of another type, grain boundary corrosion rates in a [100] series of aluminum bicrystals are to be measured as a function of orientation difference. This series is of a type which has been used for measuring grain boundary energies in fcc metals, thus permitting a comparison of the two properties.

#### G. Annealing of Cold Worked Metals - B. G. Ricketts

Electron transmission microscopy is being utilized to investigate the structural changes which occur in metals as a result of annealing after plastic deformation or radiation damage.

One aspect of the work concerns the competition between recovery and recrystallization in rolled high purity aluminum single crystals, as well as an attempt to clarify the mechanism of nucleation of recrystallization. This relation between recovery and recrystallization again is being considered in an experiment to determine the effects of impurities, particularly iron and silicon, on the annealing texture of heavily cold-rolled aluminum. Quantitative x-ray texture determination as well as electron microscopy is used. This study of defect structures also includes the formation and behavior of stacking faults found at extended dislocation nodes, currently in copper-base solid solution alloys.

Another area of investigation concerns the recovery from radiation damage caused by deuteron bombardment of noble metals. Bombardment is to be carried out at various temperatures between 15°K and room temperature. It is expected that electron microscope examination can be made at the temperature of bombardment and that structural changes brought about by annealing over a wide range of temperature can be studied.

#### H. Electron and Nuclear Magnetic Resonance - C. P. Slichter

The principal emphasis in both our nuclear and electron spin resonance work has been on the structure of point defects.

The nuclear double resonance technique provides greatly increased sensitivity in detecting nuclei present in small amounts. Our current studies in metal single crystals of the resonance of nuclei near to impurities will be continued. We plan to initiate other work in insulating crystals. Initially we shall attempt to detect the proton resonance of OH radicals present in low concentrations in NaCl. Dr. Miles Klein of this department is currently studying the thermal and optical properties of these centers. From the resonance viewpoint this system is ideal since many complications are absent as a result of the fact that the electric quadrupole moment of the proton is zero.

The ferromagnetism of certain insulating materials such as EuO or EuSe is thought to involve long range spin polarization of the valence band. We are studying the resonance of dilute solutions of Mn<sup>++</sup> in PbSe, in the hope of using the electron-nuclear double resonance technique to measure such an electron spin polarization at nearby Pb or Se nuclei. We also plan to continue work on the structure of color centers in alkali halide crystals. A model for the Z<sub>1</sub> center is emerging. We plan to go to studies of centers formed by irradiation at helium temperature. A new helium cryostat with thin wall ports will be necessary. It is generally thought the centers are formed in small clusters.

Initial experiments will be the measurement of the oscillator strengths of  $V_k$  and H bands and a careful search for interactions of the  $V_k$  or H with nearby imperfections.

#### I. Clustering of Impurities in Solid Solutions in Metals -

C. A. Wert

The placement of atoms in the crystal of a solid solution is probably never the ideal random arrangement. Because of forces of attraction or repulsion between solute atoms, clusters of like atoms exist in either more or less than random numbers. For alloys of oxygen and nitrogen in solid solution in the bcc metals, the attractive forces are especially large, and relatively large numbers of clusters of two, three and more atoms exist at room temperature even in dilute (i.e., less than 1 at %) solutions. These clusters diffuse through the metal at different rates and differences in their relative motion permit their existence to be determined by internal friction methods. Alloys of oxygen in niobium are being studied to determine the following properties of clusters of a few atoms: 1) relative diffusion rates, 2) binding energies per atom, 3) absolute numbers of clusters of several sizes expected at various temperatures and concentrations, and 4) configuration in the metal.

#### IV. Phase Changes and Precipitation in Alloys and Glasses

##### A. Enthalpy Changes in Athermal Solid State Transformations -

C. J. Altstetter

The development of the thermodynamic analysis of martensitic transformations is presently hampered by the lack of reliable values for the enthalpy changes of the transformations. The object of this research is to design, construct and operate a calorimeter capable of accurate measurement of latent heats but which is simple to operate and requires no machining of the specimen or mechanical constraints on the specimens.

It is believed that this can be accomplished by modifying the adiabatic calorimeter design principle to take advantage of the athermal character of the transformation. Instead of maintaining adiabatic conditions between the specimen and its enclosure by supplying accurately metered electrical energy to an internal heater in the specimen, in the proposed calorimeter a constant temperature difference between the specimen and its enclosure will be maintained. For small values of  $\Delta T$  this will result in a constant rate of heat exchange. The value of the transformation enthalpy change may then be obtained from the magnitude of the anomaly in the heating (or cooling) curve. Besides ease of operation and mechanical simplicity, this method has the advantage

that both the heating and cooling transformations may be studied. In principle the entire temperature range over which martensitic transformations occur is accessible by this method.

B. Structural Changes in Simple Glass Systems during Nucleation of Crystalline Phases - C. G. Bergeron

The primary objective of this program is a study of the structural changes which lead to the nucleation of crystalline phases in glasses. The specific glass systems under study are the lead borate and lead silicate systems.

There is some evidence to indicate that the internal nucleation of crystalline phases in certain glasses may occur as the result of liquid unmixing or the formation of two immiscible liquids. Growth of an ordered phase may subsequently proceed from the interface between the two liquids.

The work in this program is primarily concerned with the structural rearrangement occurring within the nucleation temperature range. Changes in structure will be investigated by the techniques of low-angle scattering of x-rays, electron microscopy, conventional x-ray diffraction analysis, differential thermal analysis, and measurements of electrical conductivity.

C. Diffusionless Phase Changes in non-Ferrous Metals and Alloys - T. A. Read

Work on Au-Zn, Au-Cd, and Cu-Au-Cd beta phase alloys is continuing in an attempt to learn more about the vacancy behavior in these materials. Previous work in this laboratory has shown that approximately one percent vacancies can be frozen-in in these alloys when quenched from near the melting temperature. X-ray, dilatation measurements, and electrical resistance methods are being used to determine vacancy contents, and the annealing kinetics and formation of vacancy loops during annealing is being studied by transmission electron microscopy. Methods are being devised to determine if vacancies preferentially exist on certain atomic sites, i.e., Au vs. Zn.

Solid state transformations and the role of crystalline defects in phase nucleation and growth are being studied in several materials, principally those alloys mentioned in the preceding paragraph. Transformations of interest are diffusionless (or martensitic) in nature, although it is planned to initiate studies on transformations which are classified as "massive" in nature. In addition to the CsCl to orthorhombic transformation in Au-Cd alloys and the beta-to-zeta transformation in Ag-Zn, a recent study of the similar transformation in  $\text{NH}_4\text{Cl}$  has been initiated.

Publications (for the Calendar Year 1963):

- C. G. Bergeron, C. K. Russell, and A. L. Friedberg, "Thermal Analysis of Lead Borate Glasses during Crystallization," J. Am. Cer. Soc. 46, (1963) pp. 246-247.
- Howard K. Birnbaum, "The Formation of Point Defects during Plastic Deformation and their Subsequent Annealing Behavior," J. Appl. Phys. 34, (1963) pp. 2175-2185.
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- D. R. Frankl, "Transmission Electron Microscopy of Cleaved Silicon," J. Appl. Phys., (1963) pp.
- N. Nakanishi and C. M. Wayman, "The Effect of Copper on the Martensitic Transformations in Beta Phase AuCd Alloys," Trans. AIME 227, (1963) pp. 500-504.
- R. L. Patterson and C. M. Wayman, "A Study of Contamination Rates in an Electron Microscope," Rev. Sci. Instr. 34, (1963) pp. 1213-1215.
- C. M. Wayman, K. M. Thein, and N. Nakanishi, "Quenched-in Defects in CsCl AuCd Alloys," J. Appl. Phys. 34, (1963) pp. 2842-2846.
- C. M. Wayman, K. M. Thein, and N. Nakanishi, "The Annealing of Quenched-in Defects in CsCl AuCd Alloys," J. Appl. Phys. 34, (1963) pp. 2847-2851.
- H. G. Drickamer and J. C. Zahner, "The Effect of Pressure on Electronic Structure," in Advances in Chemical Physics (Interscience-Wiley, New York, 1963), Vol. IV, pp. 161-200.
- H. G. Drickamer, "The Electronic Structure of Solids Under Pressure," in Solids Under Pressure (McGraw-Hill Book Co., 1963), pp. 357-385.
- H. G. Drickamer, "The Use of Pressure to Investigate the Electronic Structure of Ionic Crystals," in Physics and Chemistry in Ceramics (Gordon and Breach, 1963), pp. 131-146.
- H. G. Drickamer, "The Approach to the Metallic State at High Pressure," in Physics and Chemistry of High Pressure (Staples Printers, London, England, 1963), pp. 122-128.

- H. G. Drickamer, "Some Possible Fixed Points for Calibration Above 100 Kilobars," in High Pressure Measurement (Butterworths, London, 1963), pp. 34-39.
- H. G. Drickamer and R. A. Stager, "Ytterbium: Effect of Temperature and Pressure on Resistance," Science 139, (1963) pp. 1284-1285.
- H. G. Drickamer and R. B. Aust, "Carbon: A New Crystalline Phase," Science 140, (1963) pp. 817-819.
- H. G. Drickamer and B. M. Riggelman, "The Approach to the Metallic State as Obtained from Optical and Electrical Measurements," J. Chem. Phys. 38, (1963) 2721-2725.
- H. G. Drickamer and R. A. Stager, "The effect of Temperature and Pressure on the Resistance of Four Alkaline Earth Metals," Phys. Rev. 131, (1963) pp. 2524-2527.
- H. G. Drickamer and R. A. Stager, "The Effect of Temperature and Pressure on the Resistance of Four Alkali Metals," Phys. Rev. 132, (1963), 124-128.
- H. G. Drickamer and S. Minomura, "The Effect of Pressure on the Resistance of some Transition Metal Oxides and Sulfides," J. Appl. Phys. 34, (1963) pp. 3043-3049.
- H. G. Drickamer, "Pressure and Electronic Structure," Science 142, (1963), pp. 1429-1435.
- Miles V. Klein, "Phonon Scattering by Lattice Defects," Phys. Rev. 131, (1963) pp. 1500-1510.
- K. H. Bennemann, "General Method for Determining Lattice Point Defect Configurations Including their Dependence on Electron Redistribution," Phys. Rev. 130, (1963) pp. 1757-1762.
- K. Herschbach, "Isothermal Annealing of Deuteron-Irradiated Al and Au below 60°K," Phys. Rev. 130, (1963) pp. 554-564.
- R. O. Simmons and R. W. Balluffi, "Measurement of Equilibrium Concentrations of Vacancies in Copper," Phys. Rev. 129, (1963) pp. 1533-1544.
- R. W. Balluffi, J. S. Koehler, and R. O. Simmons, "Present Knowledge about Point Defects in Deformed Face-Centered-Cubic Metals," in Recovery and Recrystallization of Metals, ed. by L. Himmel (Interscience, 1963), pp. 1-62.

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R. O. Simmons, "Properties of Vacancies in the Noble Metals," J. Phys. Soc. Japan 18, (1963) Suppl. II, pp. 172-178.

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J. A. Venables, "A Liquid Helium Cooled Tilting Stage for an Electron Microscope," Rev. Sci. Instr. 34, (1963) pp. 582-583.

J. A. Venables, Comments on "A Dislocation Model for Twinning in fcc Metals," Acta Met. 11, (1963) p. 1368.

M. de Jong and J. S. Koehler, "Annealing of Pure Gold Quenched from above 800°C," Phys. Rev. 129, (1963) pp. 49-61.

M. de Jong and J. S. Koehler, "Diffusion of Single Vacancies and Divacancies in Quenched Gold," Phys. Rev. 129, (1963) pp. 40-49.

F. Dworschak, K. Herschbach, and J. S. Koehler, "Stage-III Annealing of Proton-Irradiated Noble Metals," Bull. Am. Phys. Soc. 8, (1963) p. 519.

D. Lazarus, "High Pressure Studies of Point Defects," J. Phys. Soc. Japan 18, (1963) Suppl II, pp. 224-228.

C. P. Flynn and R. L. Odle, "Long Range Electron Density Oscillations at Non-Zero Temperatures," Proc. Phys. Soc. 81, (1963) pp. 412-415.

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C. H. Neuman, "Internal Friction in Quenched Au," Bull. Am. Phys. Soc. 8, (1963) p. 237.

F. M. Lurie and C. P. Slichter, "Spin Temperature in Nuclear Double Resonance," Phys. Rev. Letters 10, (1963) pp. 1403-1405.

H. Blum, "Question of the Paramagnetism of the M Center in Sodium Fluoride," Phys. Rev. 128, (1963) p. 627.

Charles P. Slichter, "Magnetic Resonance Studies of F and M Centers," J. Phys. Soc. Japan 18, (1963), Suppl. II, pp. 254-255.

A. C. Anderson and R. J. Sarwinski, "Remanent Magnetic Fields in Nb-Zr Superconducting Solenoids," Rev. Sci. Instr. 34, (1963) pp. 298-299.

A. C. Anderson, W. Reese, and J. C. Wheatley, "Specific Heat, Entropy, and Expansion Coefficient of Liquid He-3", Phys. Rev. 130, (1963) 495-501.

A. C. Anderson, W. Reese, and J. C. Wheatley, "Properties of He<sup>3</sup> at Pressures Greater than the Minimum in the Melting Curve," Phys. Rev. 130, (1963), pp. 1644-1653.

A. C. Anderson, W. Reese, and J. C. Wheatley, "Thermal Conductivity of some Amorphous Dielectric Solids Below 1°K," Rev. Sci. Instr. 34, (1963), pp. 1386-1390.

Publications (for the Calendar Year 1962) which were omitted from the report of AEC-supported research for 1962-1963.

Walter Bauer, John W. DeFord, James S. Koehler, and John W. Kauffman, "Low-temperature Annealing Spectrum of Electron-Irradiated Gold and Cadmium," Phys. Rev. 128, (1962) pp. 1497-1505.

J. R. Parsons, R. W. Balluffi, and J. S. Koehler, "Direct Observation of Neutron Damage in Germanium," Appl. Phys. Letters 1, (1962), pp. 57-58.

D. Lazarus, "Mass Dependence of Intermetallic Diffusion," in Radioisotopes in the Physical Sciences and Industry (Intl. Atomic Energy Agency, Vienna, 1962), pp. 160-168.

D. Lazarus and J. Bass, "Effect of Pressure on Mobility of Interstitial Carbon in Iron," J. Phys. Chem. Solids 23, (1962) pp. 1820-1822.

C. P. Flynn, "Linde's Law and the Scattering Power of Associated Point Defects," Phys. Rev. 126, (1962) pp. 533-537.

C. P. Flynn, "Vacancies and Complexes in the Noble Metals," Phys. Rev. 125, (1962) pp. 881-895.

C. P. Flynn, "The Residual Resistivity Due to Point Defect Pairs," J. Phys. Radium 23, (1962) pp. 654-658.

A. C. Anderson, W. Reese, and J. C. Wheatley, "Magnetic Properties of He-3 at Low Temperatures," Phys. Rev. 127, (1962) pp. 671-681.

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H. G. Drickamer, R. A. Stager and A. S. Balchan, "A High Pressure Phase Transition in Metallic Tin," J. Chem. Phys. 37, (1962) pp. 1154-1155.

H. G. Drickamer and G. A. Samara, "The Effect of Pressure on the Resistance of PbS and PbTe," J. Chem. Phys. 37, (1962) pp. 1159-1160.

H. G. Drickamer, S. Minomura and G. A. Samara, "The Temperature Coefficient of Resistance of the High Pressure Phases of Si, Ge, and Some III-V and II-VI Compounds," J. Appl. Phys. 33, (1962) pp. 3196-3198.

H. G. Drickamer and R. E. Tischer, "The Use of Pressure to Investigate Local Symmetry and Compressibility of Glass," J. Chem Phys. 37, (1962) pp. 1554-1562.

Contract: IBM Corporation, Yorktown Heights, New York

Contract Number: AT(30-1)-2811

Present Contract Term: May 15, 1964 through May 14, 1965

Cost to AEC: \$52,400

Contract Title: DEFECTS IN CRYSTALS

Investigators: Arthur S. Nowick

#### Scope of Work:

A continued study of point defect phenomena in crystals will be carried out by techniques which are capable of distinguishing among the various types of defects. These techniques include anelastic relaxation studies in metallic alloys and in elemental and possibly compound semiconductors containing defects or impurities in low concentrations. The work on alloys will continue to emphasize the use of the Zener relaxation to detect small supersaturations of vacancies. The work on semiconductors, on the other hand, will attempt to determine the defect symmetry (and therefore, the sites of the defects) from the relaxations which occur. The theory of relaxation phenomena, which has already been developed using group representation theory, will be further extended. Finally, direct determination of the equilibrium density of defects in alkali metals and dilute alloys will be undertaken using precision X-ray and dilatometric techniques with the principal aim of studying vacancy-solute interactions.

Among the major accomplishments to date are: a) development of a theory which determines the occurrence of dielectric and anelastic relaxation in terms of the local symmetry of the defect and the symmetry of the crystal in which it resides; b) the investigation by anelastic techniques of the annealing out of vacancies in a Ag-Zn alloy at extremely dilute concentrations (mole fractions from  $10^{-11}$ ); c) discovery of an internal friction peak due to the vacancy-impurity pair in alkali halides; d) discovery of a new phenomenon, the anelastic piezo-resistance effect, which is the change in resistivity due to the reorientation of defects under an applied stress.

#### Recent Publications:

R. W. Dreyfus, "Preparation of Alkali Halide Crystals," Chapter 21 of the book, The Art and Science of Growing Crystals, ed. J. J. Gilman, Published by John Wiley and Sons, 1963.

R. W. Dreyfus, "Ionic Conductivity and Dielectric Relaxation in  $KCl:SmCl_2$  and  $NaCl:SmCl_2$ ," Bull. Am. Phys. Soc. 8, (1963) p. 268.

Recent Publications: continued

R. B. Laibowitz and R. W. Dreyfus, "Zener Relaxation in Mixed Ionic Crystals," Bull. Am. Phys. Soc. 8, (1963) p. 268.

R. W. Dreyfus, "Study of Doped Alkali Halide Crystals by Dielectric and Anelastic Relaxation," Bull. Am. Phys. Soc. 8, (1963) p. 253.

Contract: Johns Hopkins University, Baltimore, Maryland

Contract Number: AT(30-1)-2185

Present Contract Term: June 1, 1964 through May 31, 1965

Cost to AEC: \$44,951

Contract Title: X-RAY SPECTROSCOPY

Investigators: J. A. Bearden

#### Scope of Work:

Previous theoretical and experimental work at Johns Hopkins University has shown that the ruled grating wavelengths are subject to large corrections and errors. Density and x-ray diffraction measurements on single crystals of silicon, combined with a precision value of Avogadro's number have provided the best determination of the ratio of the x unit to the Angstrom. These measurements will be continued with other selected crystals.

The ratio of five x-ray wavelength standards has been determined with calcite, silicon and quartz crystals with an apparent accuracy of 1 ppm. A new series of measurements is planned, using more carefully selected crystals and improved x-ray techniques. This experiment is primarily designed to test the precision as indicated in the above measurements and establish a measure of the maximum precision that can be attained with present x-ray experimental techniques.

The fine structure associated with the high frequency limit of the continuous x-ray spectrum for some elements has been theoretically attributed to solid state effects. The mercury gas target x-ray tube did not exhibit structure, but solid state mercury has never been analyzed. Measurements on solid mercury will be undertaken. The tungsten high frequency limit has the most pronounced structure measured to date, and tungsten carbonyl in gas form will be measured.

The application to the double crystal spectrometer method and recently developed precision wavelength techniques to the problem of small angle scattering will be made. A reduction in the magnitude of the corrections which currently must be applied to small angle scattering would improve interpretations and possibly extend the use of this method to other important problems.

Use of the new x-ray wavelength tables will be made in a study of the  $L_{III}$ - $L_{II}$  and  $L_{III}$ - $L_I$  atomic level separation of selected elements. Also a study  $^{III}$  of x-ray excitation as a function of the part of the x-ray line used to indicate ionization will be made.

Recent Publications:

Alan J. Bearden, F. N. Huffman, "Precision Measurements of the Cleavage Plane Grating Spacing of Potassium Acid Phthalate," Review of Scientific Instruments 34, (1963) p. 1233.

Contract: Kansas, University of, Lawrence, Kansas

Contract Number: AT(11-1)-1197

Present Contract Term: June 1, 1964 through May 31, 1965

Cost to AEC: \$41,000

Contract Title: POINT DEFECTS IN IONIC CRYSTALS

Investigators: Robert J. Friauf

Scope of Work:

Diffusion measurements for both Tl and Cl in TlCl have been extended to temperatures near the melting point. Observed activation energies are 0.77eV  $D_i^*/D_i$ , are 0.015 to 0.051 for Tl and 0.73 to 0.66 for Cl at temperatures of 280° to 410°C. The sum of  $f_{Tl} + f_{Cl}$  is greater than the theoretical value for free vacancies, namely  $f_v = 0.653$ , at all temperatures. If the total discrepancy is attributed to diffusion by neutral vacancy pairs, the vacancy pair contribution varies from 15% to 280° to 10% at 410°C. Another possible explanation is that ions may be able to jump into a vacancy from next nearest neighbor as well as nearest neighbor positions. Experiments are underway to measure conductivity and diffusion in TlCl doped with Pb in order to obtain an independent measurement of the transport numbers for the two kinds of ions.

Diffusion measurements for Ag in AgCl are in progress in the temperature range from 300° to 420°C. The experimental correlation factor is  $f_{Ag} = 0.40$  to 0.50 for the measurements already obtained. These values indicate that both collinear and non-collinear interstitialcy processes must occur for Ag ions. A detailed analysis will be made when complete results are available.

Diffusion measurements for Na in NaCl are in progress in the temperature range from 575° to 725°C. The Na diffusion values are in good agreement with the total ionic conductivity after the correlation factor for free vacancies is included. Thus there is no indication at present of a large contribution from neutral vacancy pairs. The measurements need to be extended to a greater temperature range and to purer materials.

Computer calculations of correlation coefficients are contemplated for circumstances such as those encountered above in which a single ion may participate in several different kinds of jumps. Diffusion experiments may be carried out with an applied electric field in NaCl or TlCl, or to study isotope effects in NaCl or AgCl.

Recent Publications:

R. J. Friauf, "Ionic Conductivity and Diffusion in Ionic Crystals," Am. Inst. of Physics Handbook, 2nd Ed., D. E. Gray, editor, (McGraw-Hill Book Co., Inc. New York, 1963), Sec. 9, pp. 63092.

G. E. Conklin and R. J. Friauf, "Electron Spin Resonance of the  $Z_1$  Band in KCl with  $SrCl_2$ ," Phys. Rev. 132, (1963) pp. 189-194.

F. Pilcher, D. Schinke, and R. J. Friauf, "Optical Absorption of Color Centers in Lithium Fluoride containing Magnesium Additive," J. Phys. Chem. Solids 24, (1963) pp. 1687-1691.

Contract: Kent State University, Kent, Ohio

Contract Number: AT(11-1)-1374

Present Contract Term: June 15, 1964 through June 14, 1965

Cost to AEC: \$17,308

Contract Title: GENERAL STUDY OF LOCAL SYMMETRY BONDING IN NON-CENTROSYMMETRIC SYSTEMS BY ELECTRON PARAMAGNETIC RESONANCE TECHNIQUES

Investigators: Stanley H. Christensen

Scope of Work:

The first goal of this project is the construction of a high-sensitivity, X-band, paramagnetic resonance spectrometer. This spectrometer will utilize a 500 mw klystron, frequency-stabilized on a reference cavity, and will have a microwave bridge with balanced bolometer detection.

Using this spectrometer, studies will be undertaken of Stark shifts, linear in an applied electric field, in the paramagnetic resonance spectrum of iron-group ions in non-centrosymmetric crystalline environments.

The basic research goals are two-fold:

- 1) To study the mechanisms causing Stark shifts;
- 2) To utilize these shifts in an effort to study local environmental features such as the degree of covalent bonding or distortions from full substitutional symmetry produced by strains, stacking faults, vacancies, or influences of covalent bonding.

The early work of this program will be concentrated on the first of these goals, particularly in an effort to understand the angular dependence and magnitude of the shifts as they relate to the local symmetry, to the degree of covalency, and to other paramagnetic resonance features such as the relaxation time,  $T_1$ . It is intended to begin these studies with divalent copper in nearly tetrahedral local symmetries.

Contractor: Arthur D. Little, Inc., Cambridge, Massachusetts

Contract Number: AT(30-1)-2756

Present Contract Term: April 15, 1963 through April 14, 1964

Cost to AEC: \$49,880

Contract Title: ROLE OF LATTICE IMPERFECTIONS IN BEHAVIOR OF SOLIDS

Investigators: Richard S. Davis

Scope of Work:

Surface reactions on solids are being studied in two areas:

1. the interaction of surfaces with their environment, with particular emphasis on oxidation, and
2. the interaction of lattice vacancies with surfaces.

A new technique has been developed by which the oxide formed on aluminum can be studied directly in the electron microscope. A number of new observations have been made, particularly with respect to the mechanism of oxidation. The low temperature ( $< 450^{\circ}\text{C}$ ) amorphous oxide was found to grow by the transport of metal ions, whereas the high temperature ( $> 450^{\circ}\text{C}$ ) crystalline oxide was found to grow by the transport of oxygen ions. This work is being extended to aluminum base alloys. Low energy electron diffraction equipment is also being constructed so that the very early stages of oxidation can be studied. In this way the oxidation process will be observed starting with a clean metal surface.

The interaction of vacancies with surfaces is studied by observing the nucleation of pits which form during cooling from elevated temperatures on electropolished surfaces of aluminum single crystals. The pits nucleate as a result of the supersaturation of vacancies which occurs during cooling. The theoretical expression for the temperature dependence of the nucleation process has been derived and experimentally measured, with excellent agreement. The data leads to an experimentally measured average dislocation core energy of  $1.2 \times 10^{-5}$  ergs per cm.

Recent Publications:

P. E. Doherty and R. S. Davis, "Direct Observation of the Oxidation of Aluminum Single-Crystal Surfaces," J. of Appl. Physics, 34, (1963) p. 619.

P. E. Doherty and R. S. Davis, "Condensation of Vacancies in Aluminum at the Metal-Oxide Interface," Conference on Clean Surfaces, NY Acad. of Sciences, 101, (1963) p. 787.

Contract: Little, Arthur D., Inc., Cambridge, Massachusetts

Contract Number: AT(30-1)-3411

Present Contract Term: June 15, 1964 through June 14, 1965

Cost to AEC: \$29,330

Contract Title: INVESTIGATION OF DEFORMATION OF TRANSITION METAL  
CARBIDES AND BORIDES AT HIGH TEMPERATURES

Investigators: D. W. Lee

Scope of Work:

Preparation and characterization of suitable specimens for mechanical property measurements will be undertaken. Single crystal and large grain size polycrystals of ZrC and ZrB<sub>2</sub> will be prepared by a zone melting technique previously developed at Arthur D. Little, Inc. High purity materials having a controlled range of stoichiometry can be prepared by this technique. Vacuum and protective atmosphere hot pressing will be utilized to obtain fine grain size high density materials. All specimens will be well characterized, both physically and chemically.

High temperature differential creep measurements will be made in compression on selected samples in order to determine and delineate the stress and temperature dependence of the creep rate and creep fracture in single and polycrystalline material, grain size effects in polycrystalline samples and the influence of lattice defects (stoichiometry) on the creep rate. The temperature range to be covered is anticipated to be 1500°C - 2200°C.

Characterization of specimens before and after deformation studies will include extensive microstructure studies to define structural changes which have taken place. Methods for revealing dislocation networks and changes in dislocation structure will be developed. Microstructural observation will be correlated with the phenomenological studies.

The information obtained from this study will permit one to ascertain the rate controlling process in these materials under specific conditions. The knowledge may suggest methods of influencing the deformation and strength through solid solution alloying, changes in defect concentration or second phase dispersion.

Contract: Litton Systems, Inc., St. Paul, Minnesota

Contract Number: AT(11-1)-722

Present Contract Term: February 15, 1964 through February 14, 1965

Cost to AEC: \$57,289

Contract Title: SURFACE BOMBARDMENT STUDIES

Investigators: Gottfried K. Wehner

Scope of Work:

1. Sputtering of Single Crystals - The objective of this project is to obtain information on correlated atomic collision sequences, their relative importance in various crystals, the positions of surface atoms, and the annealing rates of radiation damage. The interpretation of the results is invaluable for a basic understanding of sputtering and of radiation damage. These objectives are being accomplished by the sputtering of single crystals by ion bombardment which generally results in a pronounced atom ejection in certain preferred directions. The directions in which momentum is focused have been investigated for fcc, bcc, hcp metals and the diamond and zinc blende structures. Non-normal surface atom positions have been determined in some cases and the annealing rates of the damage produced by ion bombardment in diamond and zinc blende structures have been studied in detail.

2. Sputtering Yield Measurements with Mass Separated Hydrogen Beams - In past work we have measured the sputtering yields of 18 metals under bombardment by 3-10 kev molecular hydrogen ions  $H_2^+$  and  $H_3^+$ . We plan to extend this survey to  $H^+$  and the analogous deuterium ions. These data are of direct relevance to the evaluation of wall materials for thermonuclear power devices and are, furthermore, important for the verification of theories of the relatively simple case of sputtering by light, fast ions. Drilling holes in thin metal foils by mass-analyzed, intense beams have been and will be employed with modified ion source and gas supply. This technique gives 3% precision and is self-corrected for the equilibrium roughness of the surface encountered in a practical thermonuclear power device.

Recent Publications:

G. S. Anderson, "Atom Ejection in Low Energy Sputtering of Single Crystals of bcc Metals," J. of Appl. Physics, Vol. 34, No. 3, (1963) pp. 659-663.

Contractor: Louisiana State University, Baton Rouge, Louisiana

Contract Number: AT(40-1)-3087

Present Contract Term: February 15, 1964 through February 14, 1965

Cost to AEC: \$46,013

Contract Title: CONDUCTIVITY TENSORS IN METALS AND SEMICONDUCTORS

Investigators: J. M. Reynolds

Scope of Work:

The electrical magnetoresistance, the Hall effect, the thermal magnetoresistance, the Righi-Leduc effect, the thermoelectric effect, the Ettingshausen-Hernst effect, the Peltier effect and the Ettingshausen effect will be accurately measured in single crystals of several metals and semiconductors. These measurements will be made for various crystallographic orientations at temperatures throughout the liquid helium range (also at liquid hydrogen temperatures when needed) and in magnetic fields from zero up to 60 kilogauss. The data obtained will be used to construct the complete electrical, thermal, and thermoelectric tensors for each material. From these tensors the conductivity tensor elements (kinetic coefficients) will be calculated and compared with those computed from transport theory. Among the metals to be studied are magnesium, cadmium, tin, antimony, and bismuth. Measurements are also planned on indium antimonide, and indium arsenide. Other studies, such as electron tunneling experiments, which are related to various aspects of the quantum transport theories, will be carried out.

Recent Publications:

N. H. Zebouni, J. M. Reynolds, and C. G. Grenier, "Electron Transport Phenomena in Zinc at Liquid Helium Temperatures," Phys. Rev. 129, (1963) p. 1088.

J. M. Reynolds, J. R. Sybert and C. G. Brenier, "Electron Transport Phenomena in Bismuth at Liquid Helium Temperatures," Phys. Rev. 132, (1963) p. 58.

N. H. Zebouni, R. E. Hamburg, and H. J. Mackey, "Magnetomorphic Oscillations in the Hall Effect and Magnetoresistance in Cadmium," Phys. Rev. Letters 11, (1963) p. 260.

J. M. Reynolds, G. N. Rao, C. G. Grenier, and N. H. Zebouni, "Galvanomagnetic Effects in Antimony at Liquid Helium Temperatures," To be published in Phys. Rev. (January, 1964)

SUPPORTING AGENCY:

Atomic Energy Commission

TITLE OF PROJECT:

Electron Spin Resonance and Optical Absorption in Compacted Vitreous Silica

Give names, departments, and official titles of PRINCIPAL INVESTIGATORS and ALL OTHER PROFESSIONAL PERSONNEL engaged on the project.

Dr. David G. Keiffer, Associate Professor, Physics Department

# 15,143

NAME AND ADDRESS OF INSTITUTION:

Loyola University, New Orleans, Louisiana 70118

SUMMARY OF PROPOSED WORK - (200 words or less. Omit confidential data.) - In the Science Information Exchange summaries of work in progress are exchanged with government and private agencies supporting research, and are forwarded to investigators who request such information. Your summary is to be used for these purposes.

The purpose of this work is to study the effects of ionizing radiation on vitreous silica that has been compacted by compressing it to pressures of 100,000 atmospheres. Previously published work showed that the radiation rapidly decreased the density of compacted silica. A preliminary experiment also showed that the radiation-induced paramagnetic defect concentration is much larger in compacted silica than in normal silica. Electron spin resonance and optical absorption measurements will be made to determine the relation of these defects to those previously found in uncompact high purity silica. The defect concentration will be measured as a function of irradiation dose and irradiation temperature in an effort to determine what part these defects play in the rapid expansion of compacted silica subjected to ionizing radiation.

Period for this NRP

11	-64	td	0	-65
MO	YR	MO	YR	

Sub-group

SIGNATURE OF  
PRINCIPAL  
INVESTIGATOR

Identify the Professional School (medical, dental, public health, graduate, or other) with which this project should be identified:

SCHOOL Arts and Sciences

INVESTIGATOR — DO NOT USE THIS SPACE

PROJECT NO. 25,294  
The purpose this year:

NOT FOR PUBLICATION OR  
PUBLICATION REFERENCE

Division of Research  
United States Atomic Energy Commission

REPORTING AGENCY:

TITLE OF PROJECT:

**Defect Structures in Nonstoichiometric Oxides**

Give names, departments, and official titles of PRINCIPAL INVESTIGATORS and ALL OTHER PROFESSIONAL PERSONNEL engaged on the project.

**Robert N. Flumerthal, Principal Investigator**  
Associate Professor, Mechanical Engineering

# 25,294

NAME AND ADDRESS OF INSTITUTION:

**Marquette University**

SUMMARY OF PROPOSED WORK -- (Approximately 200 words. Omit confidential data.) In the Science Information Exchange summaries of work in progress are exchanged with government and private agencies supporting research, and are forwarded to investigators who request such information. Your summary is to be used for these purposes. Please make your summary substantive in nature, rather than generally descriptive.

The purpose of the proposed research is to obtain information regarding the defect structure (i.e. the predominate type of atomic and electronic defects present and the equilibrium relationships between them) in nonstoichiometric oxides from their electrical and thermodynamic behavior. These types of measurements also furnish information regarding the energy necessary to form the various atomic and electronic defects which together constitute the defect structure of a nonstoichiometric oxide.

In this study, either an electrochemical cell technique or a gas equilibrium method will be utilized to obtain relative partial molar free energies, entropies and enthalpies of oxygen and the partial pressure of oxygen for nonstoichiometric oxides as a function of temperature and composition. Ionic transport measurements employing an emf method will be made on these nonstoichiometric oxides which indicate the presence of a significant ionic contribution to conduction. For these oxides, the ionic transport number will be determined as a function of  $P_{O_2}$  and temperature. The electrical conductivity of the nonstoichiometric oxide specimens (single crystals, if available) will be measured as a function of temperature, oxygen partial pressure and composition.

Period for this NRP

1-65 to 12-65

MO YR MO YR

Sub-group

SIGNATURE OF  
PRINCIPAL  
INVESTIGATOR

Identify the Professional School (medical, dental, public health, graduate, or other) with which this project should be identified:

SCHOOL College of Engineering

**Contract:** Maryland, University of, College Park, Maryland

**Contract Number:** AT(40-1)-2068

**Present Contract Term:** March 15, 1964 through March 14, 1965

**Cost to AEC:** \$14,994

**Contract Title:** PROCESSES OF DIFFUSION AND ELECTRICAL CONDUCTION  
IN SOLIDS

**Investigators:** Homer W. Schamp, Jr.

**Scope of Work:**

A continuation of measurements in progress on self-diffusion coefficients in the alkali halides at high temperatures and pressures is proposed. The range of the measurements is from 650° C to 900° C, and the pressure range will extend to at least 30 kilobars. Measurement of the chloride ion diffusion coefficient in sodium chloride will be made. The effect of length of time of the diffusion anneal on this diffusion coefficient will be investigated. The diffusion coefficient will be investigated. The diffusion coefficient of the chloride ion in potassium chloride at 790° C will be reexamined since it showed some anomalous behavior in the measurements already made. Attempts will be continued to measure the ionic conductivity of the alkali halides as a function of temperature and pressure.

**Recent Publications:**

- J. N. Mundy and E. Rapoport, "Use of Melting Points for Measuring Pressure, High-Temperature Vessels," High Pressure Measurement (1963), Butterworth.
- J. N. Mundy and E. Rapoport, "Anionic Self-Diffusion in Potassium Chloride at High Pressures and High Temperatures", Bull. Am. Phys. Soc. 8, 89, (1963).

**Contractor:** Massachusetts Institute of Technology, Cambridge, Mass.

**Contract Number:** AT(30-1)-1002, Scope I

**Present Contract Term:** September 1, 1963 through August 31, 1964

**Cost to AEC:** \$64,250

**Contract Title:** THERMODYNAMIC AND OTHER ASPECTS OF METALLIC SYSTEMS

**Investigators:** M. B. Bever

**Scope of Work:**

This research is concerned with (1) the effects of deformation and annealing on the properties of metals and (2) the thermodynamics of metallic systems. Specialized equipment used consists of a liquid metal solution calorimeter, a constant temperature gradient calorimeter, and apparatus for deformation and annealing below room temperature, resistance measurements, and internal friction measurements.

(1) Deformation and Annealing - Investigations of the effects of explosive loading on the ordered and disordered alloy  $\text{Cu}_3\text{Au}$  and of the annealing kinetics of an explosively loaded gold-silver alloy have been completed. The effects of deformation and annealing below room temperature on gold and gold-silver alloys are being investigated. Preliminary measurements of the stored energy in deformed intermetallic compounds have been made; this is part of the research program on the effect of variables on the stored energy of cold work.

(2) Thermodynamics - In a continuing investigation of the heats of solution in liquid tin, bismuth, and tin-bismuth alloys, the heat of solution of selenium in bismuth has been measured recently. The energy difference between crystalline and amorphous selenium and the heat formation of  $\text{Bi}_2\text{Se}$  have also been measured and the glass transition temperature of selenium has been investigated. Measurements in earlier periods include the heats of formation of III-V compounds, the intermediate phases in the gold-tin system and solid solutions in the Au-Ag, Cu-Ni, and Cu-Sn systems, the energy of ordering of  $\text{Cu}_3\text{Au}$ , the energy of precipitation of  $\text{Cu}_3\text{Sn}$  and the excess energy of electro-deposited silver. In the current period, the heats of formation of alloys near the composition  $\text{AgMg}$  were measured.

Recent Publications:

A. S. Appleton and M. B. Bever, "The Energy Relations in the Deformation by Torsion of a Gold-Silver Alloy," Trans. Met. Soc. of AIME, Vol. 227, (1963) pp. 365-371.

B. Roessler, D. T. Novick, and M. B. Bever, "Annealing of the Ordered and Disordered Alloy  $\text{Cu}_3\text{Au}$  after Cold Work," Trans. of the Met. Soc. of AIME, in press.

M. B. Bever, "The Stored Energy of Cold Work" Encyclopedic Dictionary of Physics, Vol. 7 ed. J. Thewlis, Pergamon Press, (1962) pp. 45-46.

M. B. Bever, "Calorimetric Investigations," Compound Semiconductors, Vol. 1, Preparation of III-V Compounds, ed. R. K. Willardson and H. L. Goering, Reinhold Publishing Corporation, (1962) pp. 498-508.

**Contractor:** Massachusetts Institute of Technology, Cambridge,  
Massachusetts

**Contract Number:** AT(30-1)-1310

**Present Contract Term:** October 15, 1963 through October 14, 1964

**Cost to AEC:** \$20,250

**Contract Title:** MECHANICAL PROPERTIES OF METALS AT LOW TEMPERATURES

**Investigators:** W. A. Backofen

**Scope of Work:**

During the past year, the study of ductile fracture in aluminum at low temperatures, conducted as a Doctorate thesis research by G. Y. Chin, was completed. The work on low-temperature deformation of copper single crystals was extended considerably in the Doctorate thesis research of Shigeo Saimoto.

Copper crystals of 001, 111, and 011 orientations, together with polycrystals, were tested in tension at 273, 162, 78, and 4.2°K. Inhomogeneity of deformation in 011 crystals has been rationalized with a strain analysis showing that minimum misfit between differently oriented regions should be expected if the regions are bounded by the observed planes of 001 type. Observations on inhomogeneity of deformation in 001 crystals and its relationship to hardening behavior are now being analyzed to develop an adequate rationale for this part of the program. It has been possible to interrelate strain hardening of 111 and 001 single crystals and polycrystalline material with arguments based on the Taylor analysis of polycrystalline deformation.

Twinning was studied in both 111 and 001 crystals under tension and compression loading at 78, 18, and 4.2°K. Consistent with a simple model based on shear in a rigid-ball assembly, only 111 crystals twinned in tension, while under compression twinning was restricted to 001 crystals.

Detailed observations were also made on the fracturing process in the various crystals. Finally, comparisons could be drawn between current results and those obtained earlier in similar work on aluminum crystals.

**Contract:** Massachusetts Institute of Technology, Cambridge, Mass.

**Contract Number:** AT(30-1)-1985

**Present Contract Term:** March 1, 1964 through December 31, 1964

**Cost to AEC:** \$3,870

**Contract Title:** KINETICS OF REACTIONS BETWEEN LIQUID METALS AND LIQUID SALTS

**Investigators:** T. B. King

**Scope of Work:**

The kinetics of reactions between liquid alloys and liquid salts are being studied. From direct rate measurements on systems involving halide salts and low melting alloys and also on systems involving silicate melts, and copper and iron alloys, it can be concluded that a slow phase-boundary reaction does not control the overall rate, but the reaction rate is controlled by the transport of a constituent in either the alloy or the salt melt.

To obtain quantitative data on transport processes in the alloys, a program of measurement of diffusion coefficients in liquid alloys was started, and included a comprehensive study of the capillary method for measuring diffusion coefficients in liquids.

The conclusions from studies of electrode kinetics in fused halides and silicates are, in general, the same as those obtained from direct rate studies. These studies have been conducted using solid platinum, silicon and carbon electrodes and a liquid iron-silicon electrode. There is no essential difference between the behavior of the liquid iron-silicon electrode and a solid silicon electrode.

Anodic and cathodic processes in silicate melts are very slow because of slow transport processes within the silicate. The electrode reactions can only be studied by techniques, applicable to fast reactions, which have been developed for studies on aqueous electrolyte studies.

Work is at present concerned with establishing a more detailed mechanism for anodic reactions involving silicon electrodes and silicate electrolytes.

Contractor: Massachusetts Institute of Technology, Cambridge,  
Massachusetts

Contract Number: AT(30-1)-2574

Present Contract Term: September 1, 1963 through August 31, 1964

Cost to AEC: \$211,375

Contract Title: STRUCTURE AND PROPERTIES OF CERAMICS AND NONCRYSTALLINE  
SYSTEMS

Investigators: W. D. Kingery and R. L. Coble

Scope of Work:

During the past year advances have been made in understanding diffusion phenomena, solid-solid kinetics, solid-liquid kinetics, vapor deposited oxides, and mechanical and electrical properties of ceramics. Diffusion measurements were completed for Al and O in  $Al_2O_3$  and for O in  $GeO_2$ . Analysis of these data and their application to solid state processes show that grain boundary phenomena are much more important in oxides than previously recognized; diffusional creep and solid state sintering data are in agreement with this view. Effects of moving boundaries, changing volumes, and liquid flow conditions have been evaluated and tested for solid-liquid reactions; detailed analysis of material diffusion in the boundary layer is in progress. Vapors of  $Al_2O_3$ , MgO, and ZnO have been deposited on low-temperature substrates and found to have only short range order by x-ray and electron diffraction. Electronic conduction in glasses indicates an electron jump mechanism, and the electrical properties of ZnO are found to differ greatly between the non-crystalline and crystalline state. Mechanical property studies of glass strength and deformation, as well as single crystal and polycrystalline deformation are in progress.

During the next year studies will continue on kinetics and microstructure development, electrical and mechanical properties of oxide glasses and crystals, and the structure and properties of non-crystalline oxides formed by vapor deposition. Research is being initiated to investigate subsolidus equilibria and the effects of dislocations and phase boundaries on electrical and mechanical properties of ceramics.

Recent Publications:

A. R. Cooper, Jr., and W. H. Goodnow, "The Examination of Density Distributions in Dry Pressed Compacts of Ceramic Powders by Radiography of Lead Grids," Bull. Am. Ceram. Soc., 41, (1962) p 760

Recent Publications: continued

A. R. Cooper, Jr., and L. E. Eaton, "Compaction Behavior of Several Ceramic Powders," J. Am. Ceram. Soc., 45, (1962) p. 97

A. R. Cooper, Jr., and W. D. Kingery, "Kinetics of Solution in High Viscosity Liquids: Sodium Chloride-Glycerol," J. Phys. Chem., 66, (1962), p. 665

A. R. Cooper, Jr., "The Effect of the Moving Boundary on Unsteady State Diffusion Controlled Dissolution or Growth of Slabs," Trans. Farad. Soc., 480, (1962) p. 2468

A. R. Cooper, Jr., "Dissolution Kinetics in Glass-Making," VI International Congress on Glass, Advances in Glass Technology, (1962) p. 217

A. R. Cooper, "Modification of the Nernst Equation," J. Chem. Phys., 38, (1963) p. 285

A. E. Paladino and W. D. Kingery, "Aluminum Ion Diffusion in Aluminum Oxide," J. Chem. Phys., 37 (3), (1962) p. 957

W. D. Kingery, "The Thermal Conductivity of Ceramic Dielectrics," Progress in Ceramic Science, Vol. 2, J. E. Burke, Editor, Pergamon Press (1962)

W. D. Kingery, "A Review of the Stress-Strain-Time-Temperature Behavior of Ceramics," Proc. A.S.T.M. Symposium on Stress-Strain-Time-Temperature Relationships in Materials, Special Technical Publication No. 325, A.S.T.M. (1962)

S. I. Warshaw and F. H. Norton, "Deformation Behavior of Polycrystalline Aluminum Oxide," J. Am. Ceram. Soc., 45, (1962) p. 479

**Contractor:** Massachusetts Institute of Technology, Cambridge, Mass.

**Contract Number:** AT(30-1)-2879

**Present Contract Term:** September 1, 1963 through August 31, 1964

**Cost to AEC:** \$109,800

**Contract Title:** ATOMIC ARRANGEMENTS AND IMPERFECTIONS

**Investigators:** B. L. Averbach and Morris Cohen

**Scope of Work:**

Atomic arrangements and thermodynamic properties are being studied in an effort to further our understanding of the theory of alloys. In particular, x-ray techniques are being used to determine the short-range order and effects associated with differences in atomic sizes in solid solutions. During the past year, measurements have been made on iron-aluminum alloys to supplement the observations previously reported on this program; the new data suggest that the short-range order contains small domains of highly ordered material. Considerable emphasis has also been placed on the measurement of the atomic displacements associated with the vibrational spectrum. The resultant Debye temperatures for Fe-Cr, Ni-Cr, and Cu-Ni alloys indicate that the assumptions of temperature independence and applicability of the rule of mixtures usually adopted in the analysis of such data are not suitable. It is evident that a better formulation of the acoustic spectrum is required and that changes of the spectrum with temperature must be considered. This work will be continued and expanded to include measurements of the pressure dependence of elastic moduli.

Work is also under way on studies of nucleation in gold-nickel alloys, on the measurement of thermodynamic properties of iron-nickel alloys, and on the determination of atomic displacements and short-range order in iron-silicon alloys.

Studies by this group on the influence of simultaneous plastic flow on self-diffusion indicate that there is a substantial increase in the self-diffusion coefficient due to concurrent plastic flow. During the past year the influence of simultaneous compressive creep on the self-diffusion of gold has been measured, and it appears that the effects are even larger than observed on iron and nickel. A careful look at the overall problem is necessary and the entire question will be reviewed.

Recent Publications:

C. R. Houska and B. L. Averbach, "Atom Arrangements in Some Iron-aluminum Solid Solutions," J. Phys. Chem. Solids 23, 1763 (1962).

C. R. Houska, "A Theoretical Treatment of Atomic Configurations Found in Some Iron-aluminum Solid Solutions," J. Phys. Chem. Solids 24, 94 (1963).

Ken-ichi Hirano, R. P. Agarwala, B. L. Averbach and Morris Cohen, "Diffusion in Cobalt-nickel Alloys," J. Appl. Phys. 33, 3049 (1962).

Ken-ichi Hirano, Morris Cohen, B. L. Averbach and N. Ujjiye, "Self-diffusion in  $\alpha$ -iron During Compressive Plastic Flow," Trans. AIME, approximate publication date August 1963.

Ken-ichi Hirano, Morris Cohen and B. L. Averbach, "Diffusion of Iron, Cobalt and Nickel in Silver," Acta Met. 11, 463 (1963).

Contractor: Massachusetts Institute of Technology, Cambridge  
Massachusetts

Contract Number: AT(30-1)-2909

Present Contract Term: February 1, 1964 through January 31, 1965

Cost to AEC: \$15,840

Contract Title: EFFECT OF RADIATION ON CRYSTAL GROWTH RATES

Investigators: Edward A. Mason and Robert C. Reid

Scope of Work:

The main objective of this investigation is to study the effect of high energy radiation on the growth rate and habit of crystals, irradiated while they grow in a supersaturated solution.

The data obtained are expected to be helpful in providing a better understanding of the mechanisms of a crystallization process, and also in exploring the possible application to various phase transition processes in industry.

Potassium chloride crystals grown from solution inside a Co-60 radiation field were found to have a lower density (1.80) than those grown in the absence of radiation (1.984). It is believed that in the crystal growth experiments under irradiation the rate is diffusion controlled. Under such conditions, dendritic or needle-like microcrystals are formed which could occlude another liquor in pockets and yield a final crystal which has a substantial void fraction.

The true effect of gamma irradiation on crystal growth kinetics in situations which are not diffusion controlled has not yet been resolved and is now being studied in our laboratory. Solutions of potassium chloride are used at the present time. Use of succinic acid and alum is contemplated for later stages.

It is also planned to study the effect of x-rays on the growth of KCl crystals from solutions into which very small amounts of additives were added.

Studies of the effect of radiation on the rate of dissolution will be initiated for comparison with the crystal growth studies.

**Contract:** Massachusetts Institute of Technology, Cambridge, Mass.

**Contract Number:** AT(30-1)-3020

**Present Contract Term:** June 1, 1964 through May 31, 1965

**Cost to AEC:** \$6,700

**Contract Title:** X-RAY STUDY OF STRUCTURE AND DEFECTS

**Investigators:** B. E. Warren

**Scope of Work:**

A new measurement of the short-range order parameters in the alloy  $\text{Cu}_3\text{Au}$  with improvements in experimental technique and interpretation has just been completed. The new values differ considerably from the older values and they are in excellent agreement with the Cowley theory.

A major improvement has been made in the technique for the x-ray study of the structure of liquids and amorphous solids. The improvement is in the elimination of the Compton modified scattering by causing the diffraction radiation to excite fluorescence radiation in a substance so chosen that the excitation by the Compton radiation is negligible. Use of MoK $\alpha$  radiation exciting fluorescence in a yttrium compound has already been tried and found to be quite satisfactory.

For interpreting the x-ray diffraction patterns of finely divided carbon or radiation-damaged graphite, a new method has been developed for computing the complete diffraction pattern from the general Debye scattering equation. This gives completely rigorous curves for comparison with experiment.

**Recent Publications:**

Technical Report NYO-10, 106, "Single and Double Deformation Faults in Face-Centered Cubic Crystals," J. Appl. Phys. 34, (1963) p. 1973.

Technical Report NYO-10, 107, "X-Ray Profiles from Cold-Worked Metals," Acta Met. 11, (1963), p. 995.

**Contract:** Massachusetts Institute of Technology, Cambridge, Mass.

**Contract Number:** AT(30-1)-3031

**Present Contract Term:** June 1, 1964 through May 31, 1965

**Cost to AEC:** \$110,303

**Contract Title:** LOW TEMPERATURE NEUTRON PHYSICS STUDIES

**Investigators:** C. G. Shull

**Scope of Work:**

Studies of paramagnetic alignment, nuclear polarization and superconductor scattering are being carried out at low temperatures utilizing monochromatic beams of polarized neutrons. In this program, suitable crystal specimens are maintained in magnetic fields at low temperature and the neutron scattering affords information on the identification of the electron and nuclear polarization. In the latter case the scattering data can yield the nuclear spin scattering amplitudes and can bear upon the external field penetration and the hyperfine field within the crystal. Superconductor scattering effects are being sought yielding information on spin-pairing or vortex current presence in the superconducting state.

**Recent Publications:**

C. G. Shull and R. P. Ferrier, "Electronic and Nuclear Polarization in Vanadium by Slow Neutron Scattering", Phys. Rev. Letters 10, 295 (1963).

C. G. Shull, "Neutron Spin-Neutron Orbit Interaction with Slow Neutrons", Phys. Rev. Letters 10, 297 (1963).

C. G. Shull and N. S. Gingrich, "Neutron Diffraction Effects with Moving Lattices", J. Appl. Phys. (April 1964).

Contractor: Massachusetts Institute of Technology, Cambridge,  
Massachusetts

Contract Number: AT(30-1)-3134

Present Contract Term: November 1, 1962 through October 31, 1964

Cost to AEC: \$79,000

Contract Title: FUNDAMENTALS OF DIFFUSION

Investigators: R. E. Ogilvie

Scope of Work:

There are two approaches to the study of diffusion processes: (1) the microscopic approach, and (2) the macroscopic or phenomenological approach. The latter is the area of study at the present time.

The mathematical approach being used in the study of the Au-Ag-Cu system is that of Onsager. Diffusion couples have been prepared and analysed with the Electron Microanalyzer. The activity data which is necessary for the solution of Onsager's equation is being measured with a Zirconia cell. The aim of this work is to evaluate the phenomenological coefficients  $L_{ij}$  and in particular to verify the Onsager reciprocal relation, that is,  $L_{ij} = L_{ji}$ .

Diffusion of Zn along pure edge dislocations in silver bicrystals (  $[211]$  tilt axis) has been measured with the Electron Microanalyzer. The Zn has been diffused into tilt boundaries of  $8^\circ$  and  $16^\circ$  from the vapor phase. From this data it has been possible to obtain the contribution of each dislocation to the diffusion process.

The third area of work being carried out in this program is the study of the diffusion gradients that are formed during oxidation of Ni-Pt alloys. The depletion of Ni and the enrichment of Pt has been measured with the Electron Microanalyzer.

**Contract:** Massachusetts Institute of Technology, Cambridge, Mass.

**Contract Number:** AT(30-1)-3208

**Present Contract Term:** May 15, 1964 through January 15, 1965

**Cost to AEC:** \$12,805

**Contract Title:** STUDIES ON THE DISTRIBUTION OF IMPURITIES IN SOLIDS

**Investigators:** Harry C. Gatos

**Scope of Work:**

It is the immediate aim of this investigation to attain control of the heat gradients and fluxes near the solid-melt interface during solidification under non-equilibrium conditions. Under such control it should become possible to obtain data essential in the understanding of the incorporation and distribution of impurities (and defects) in solids. For this purpose, single crystals of indium antimonide and germanium will be grown from the melt containing known impurities (tellurium, gallium, etc.) since the detection and characterization of trace impurities in these materials is possible by various means including electrical measurements. In parallel to the experimental program, an attempt will be made to develop a mathematical model for the solid-melt interface under non-equilibrium conditions.

**Contract:** Massachusetts Institute of Technology, Cambridge, Massachusetts

**Contract Number:** AT(30-1)-3226

**Present Contract Term:** May 15, 1964 through May 14, 1965

**Cost to AEC:** \$34,850

**Contract Title:** RELATION OF STRUCTURAL DEFECTS AND MICROSTRUCTURE TO SUPERCONDUCTIVITY

**Investigators:** George W. Pearsall and Robert M. Rose

**Scope of Work:**

The properties of superconductors are influenced by the arrangements of atoms in the superconducting phases and the arrangements of phases in superconducting microstructures. We study the role played by imperfections in these arrangements: imperfections both in the lattice of a phase (an inter-metallic compound in our investigation) and in the phase morphology of a simple, two-phase microstructure.

Our investigation of vacancies in  $Nb_3Sn$  during the present contract year has indicated, both from experimental measurements and a theoretical analysis, that superconductivity in defect- $Nb_3Sn$  is inhibited much more by vacancies in niobium sites than by vacancies in tin sites. We shall attempt to relate these results to the bonding in this compound in order to develop a more general understanding of the influence of atomic environment in superconductors. We propose to extend this study to  $Ta_3Sn$  and to another class of compounds, probably those with NiAs-like structures.

Our measurements of superconducting properties of directionally solidified Pb-Sn eutectics indicated that the multiple connectivity between the lead-rich phase domains is the dominant imperfection affecting magnetization behavior. In order to make more perfect two-phase microstructures, with less connectivity and with more precisely controlled phase morphology, we propose to extend this study to Pb-Ag composites.

**Contract:** Massachusetts, University of, Amherst, Massachusetts

**Contract Number:** AT(30-1)-3003

**Present Contract Term:** May 1, 1964 through April 30, 1965

**Cost to AEC:** \$11,880

**Contract Title:** STUDIES OF CRYSTAL ORIENTATION IN IRRADIATED CRYSTALLINE POLYMERS

**Investigators:** Richard S. Stein

**Scope of Work:**

Films of radiation-crosslinked polyethylene have been prepared and characterized to some extent by stress-strain measurements above their melting points, microscopic examination, light-scattering, birefringence and transmission between crossed polaroids. More complete characterization by these techniques will be carried out for samples crystallized under isothermal conditions in order to better determine the effect of crosslinking and orientation above the melting point upon crystallization kinetics and morphology and to determine the mechanical and optical properties of the resultant films. At low elongations, it is known that the spherulitic morphology is predominant. The spherulites are postulated to be composed of lamella possession folded-chain crystal structure, much like with solution-grown polymer single crystals. It is believed that the degree of such chain folding decreases with elongation of such an oriented network with an increase in growth of "fringed fibril" type crystals. It is hoped to accumulate experimental evidence for such a transformation and to determine its effect upon properties.

It is also hoped to demonstrate that the rates of crystallization for the two types of crystals are affected differently by strain of the crosslinked melt.

**Recent Publications:**

K. Sasaguri, M. G. Rhodes, and R. S. Stein, "Spherulite Deformation in Polybutene-1," Polymer Letters, Vol. 1, (1963), pp. 571-574.

Contractor: Mellon Institute, Pittsburgh, Pennsylvania

Contract Number: AT(30-1)-2684

Present Contract Term: November 1, 1963 through October 31, 1964

Cost to AEC: \$130,000

Contract Title: ALLOYS OF THE NOBLE METALS

Investigators: T. B. Massalski

#### Scope of Work:

Certain aspects of the relationship between the electronic structure of alloy phases, their stability, and their physical properties will be studied experimentally and theoretically.

Temperature dependence of lattice spacings in several close-packed hexagonal Cu-Ge alloys will be established both above and below room temperature in order to study possible electron overlaps across the Brillouin zone gaps. In order to study similar effects as a function of composition lattice spacings in the h.c.p. alloys within the Ag-Au-Sn system will be determined at room temperature.

Certain aspects of martensitic transformations of the b.c.c. beta phase in the Cu-Zn system will be studied by cold-stage microscopy, particularly the slow athermal growth, the  $M_s$  temperature for bursts and the change of habit plane with composition.

The work of the plastic behavior of the h.c.p. Cu-Ge alloys will be completed with a determination of the elastic moduli and their variation with temperature. A comparison of the effect of solute atomic size and valency on the mechanical properties of the h.c.p. phases will be made for two alloy systems, Cu-Be and Ag-Sn.

The theoretical interpretation of the alpha phase electronic specific heats will be completed for the systems Cu-Zn and Ag-Sn. The electronic specific heat of very pure silver will be measured.

In order to correlate the information about the electronic structure obtained from accurate measurements of lattice spacings with a direct measurement of the density of states, intermediate-phase alloys with the close-packed hexagonal structure will be investigated.

Recent Publications:

T. B. Massalski and H. W. King, "The Lattice Spacing Relationships in H.C.P.  $\epsilon$  and  $\eta$  Phases in the Systems Cu-Zn, Ag-Zn, Au-Zn and Ag-Cd," Acta Metallurgica, Vol. 10, (1962) p. 1171

T. B. Massalski, "Letter to the Editor on Lattice Spacings in the Ag-Al System," Acta Metallurgica, Vol. 10 (1962) p. 985

T. B. Massalski, "Lattice Spacings Trends in Close-Packed Hexagonal Phases Based on the Noble Metals," Journal de Physique et le Radium, Vol. 23, (1962) p. 647

T. B. Massalski and H. W. King, "Discussion to the paper by N. F. Mott on size effects in solid solutions," Journal de Physique et le Radium, Vol. 23, (1962) p. 607

**Contract:** Michigan State University, East Lansing, Michigan

**Contract Number:** AT(11-1)-1042

**Present Contract Term:** June 1, 1964 through May 31, 1965

**Cost to AEC:** No-fund Extension

**Contract Title:** GROWTH AND PROPERTIES OF METAL AND COMPOUND  
SINGLE CRYSTALS

**Investigators:** Chuan T. Wei

**Scope of Work:**

**OBJECTIVE--**To improve the perfection of artificially prepared metal and compound single crystals and to study their mechanical and physical properties.

**REASON FOR STUDY--**Research over the past few years has made it increasingly clear that the physical and mechanical properties of crystalline solids are affected, or even determined by such imperfections as vacancies, interstitials, dislocations, and grain boundaries. The control of grain boundary imperfections by the use of single crystals, bicrystals, etc., has led to significant advances in understanding the properties of materials. The ability to produce crystals free of dislocation imperfections, and to introduce them under controlled conditions may be expected to lead to further striking advances and is the subject of this investigation.

**PROCEDURE--**Lithium fluoride and zinc single crystals are grown under controlled thermal gradients and oriented favorably for the elimination of dislocations and suppression of dislocation formation by slip. Crystal perfection and dislocations will be studied by etch pit and x-ray diffraction techniques.

**TEST OBJECTS AND AGENTS--**The initial studies are being conducted with lithium fluoride and zinc single crystals.

**ACCOMPLISHMENTS--Growth of Metal and Compound Crystals--**Using a modified Bridgman technique, zinc single crystals have been grown which are substantially free from sub-boundaries, have a dislocation density of from  $6-9 \times 10^4 \text{ cm}^{-2}$ , and show x-ray extinction over the entire surface. Using a Bridgman furnace, Li-F single crystals have been grown which have dislocation densities of from  $3-5 \times 10^4 \text{ cm}^{-2}$ . As yet dislocation free metal or compound single crystals of macroscopic size have not been grown.

**Properties of Metal and Compound Crystals--**By combining the work-hardening in the latent slip systems with the work-hardening due to reversing stresses in LiF single crystals, and yield point was increased from  $0.185 \text{ kg mm}^{-2}$  initially to  $5.40 \text{ kg mm}^{-2}$  in the latent slip systems. Such a twenty-nine fold increase is phenomenal and is being carefully studied. The results may lead to a better understanding of the work-hardening phenomena in general

**Contract:** Michigan State University, East Lansing, Michigan

**Contract Number:** AT(11-1)-1247

**Present Contract Term:** February 1, 1964 through January 31, 1965

**Cost to AEC:** \$15,111

**Contract Title:** STUDIES OF CONDUCTIVITY OF THIN METALLIC WIRES

**Investigators:** Frank J. Blatt

**Scope of Work:**

The resistivity and magnetoresistivity of thin metallic wires will be measured in the temperature range between 1.1<sup>o</sup>K and 4.2<sup>o</sup>K. Here the mean free path in the pure metals to be studied is comparable or longer than the diameters of the wires that will be used. During the previous year preliminary measurements on indium have been made. Further work on indium is contemplated, to be followed by measurements on tin and possibly gallium. The facilities that will be used are already at hand: a 15" Harvey-Wells electromagnet, sensitive millimicrovolt potentiometers, a helium research dewar, pumping lines, manometers and a manostat, and incidental equipment. There are several reasons for pursuing this work. First, it has been observed by others that the "ideal resistivity" (i.e. the temperature dependent part of the resistivity) is a function of  $\ell/d$ , where  $\ell$  is the electronic mean free path and  $d$  the wire diameter. A calculation by Blatt and Satz showed that the efficacy of electron-phonon scattering is enhanced by the proximity of surfaces that scatter electrons diffusely, and that this accounts for the observations that earlier theories had not envisaged. It was shown, also, that from such experimental work one may be able to deduce the relative magnitudes of normal and Umklapp electron-phonon scattering. We suggested that the magnetoresistance of fine wires and at low magnetic fields may be enhanced as the wire diameter is decreased. Preliminary results on indium show this very effect. From it one concludes that two types of carriers, e.g., electrons and holes, contribute to charge transport; this agrees with the conclusion of unrelated experimental work. The importance of these measurements is that accurate results on magnetoresistance of fine wires, when combined with bulk resistivity and Hall effect data, may allow the determination of the individual mean free paths of each of the two groups of carriers, rather than just their average.

**Contract:** Michigan Technological University, Houghton, Michigan

**Contract Number:** AT(11-1)-916

**Present Contract Term:** June 15, 1964 through June 14, 1965

**Cost to AEC:** \$29,914

**Contract Title:** STRUCTURE AND PROPERTIES OF SOLID SOLUTIONS

**Investigators:** A. A. Hendrickson

**Scope of Work:**

The main purpose of this investigation is to determine the cause(s) of solid solution strengthening in body-centered and face-centered cubic, solid solutions.

The body-centered cubic solutions being investigated include the Ta-Cb and Ta-V. Single crystals grown by the electron beam method are tension tested in order to determine the critical resolved shear stress and its temperature dependence. The test results are compared with current theories of the strength of body-centered cubic metals.

The face-centered cubic solid systems investigated include the Ag base Zn and Ag base Sn terminal solid solutions. Particular topics of interest are studies of strain aging phenomena, the critical resolved shear stress and its temperature dependence, and the effects of solute additions on crystal perfection.

Contractor: Michigan Technological University, Houghton, Michigan

Contract Number: AT(11-1)-1356

Present Contract Term: March 1, 1964 through February 28, 1965

Cost to AEC: \$24,553

Contract Title: DEFECT STRUCTURE IN NONSTOICHIOMETRIC OXIDES

Investigators: R. N. Blumenthal

Scope of Work:

An investigation of the electrical and thermodynamic behavior of nonstoichiometric oxides will be conducted to obtain information regarding the defect structures of these oxides. These types of measurements also furnish information regarding the energy necessary to form the various atomic and electronic defects which together constitute the defect structure of a nonstoichiometric oxide.

In this study, either an electrochemical cell technique or a gas equilibrium method will be utilized to obtain relative partial molar free energies, entropies and enthalpies of oxygen and the partial pressure of oxygen for nonstoichiometric oxides as a function of temperature and composition. Ionic transport measurements employing an emf method will be made on those nonstoichiometric oxides which indicate the presence of a significant ionic contribution to conduction. For these oxides, the ionic transport number will be determined as a function of  $P_{O_2}$  and temperature. The electrical conductivity of the nonstoichiometric oxide specimens will be measured as a function of temperature, oxygen partial pressure and composition.

NOTICE OF RESEARCH PROJECT  
SCIENCE INFORMATION EXCHANGE  
SMITHSONIAN INSTITUTION

PROJECT NO. (Do not use this space)

NOT FOR PUBLICATION OR  
PUBLICATION REFERENCE

Division of Research  
United States Atomic Energy Commission

SUPPORTING AGENCY:

TITLE OF PROJECT:

Effect of Annealing on the Substructure of Cold Worked  
fcc Metals and Alloys

List names, departments, and official titles of PRINCIPAL INVESTIGATORS and ALL OTHER PROFESSIONAL PERSONNEL engaged on the project.

Donald E. Mikkola, Dept. of Metallurgical Engineering, Assistant Professor

NAME AND ADDRESS OF INSTITUTION:

Michigan Technological University, Houghton, Michigan

SUMMARY OF PROPOSED WORK -- (Approximately 200 words. Omit confidential data.) In the Science Information Exchange summaries of work in progress are exchanged with government and private agencies supporting research, and are forwarded to investigators who request such information. Your summary is to be used for these purposes. Please make your summary substantive in nature, rather than generally descriptive.

The purpose of this proposed research is to obtain information concerning the effect of annealing on the substructure of cold worked fcc metals and alloys and the relation of changes in substructure to physical properties. Examination of the substructure will be done using X-ray diffraction techniques and also direct observation by transmission electron microscopy.

The study will involve precise analysis of the substructure during isothermal annealing of a series of fcc solid solutions such as Zn, Al or Si in Cu. Addition of elements of this type to a noble metal is known to alter the form of the substructure developed by deformation by changing the fault energy. A comparison of the changes, during annealing, of the mosaic size, microstrains and density of faults with simultaneous measurements of physical properties such as hardness and electrical resistivity will allow a definition of the property changes in terms of the structural changes. The kinetic data available for the disappearance of the defects as measured by X-rays will provide information on which processes are diffusion controlled and which occur through stress relief and dislocation glide. In addition the effect of alloying on the processes can be determined.

The next stage of the study will involve the same measurements on alloys of, for example, Ni or Ag added to Cu where the fault energy is not changed appreciably. In later stages the study will be extended to the annealing of deformed ordered alloys. The use of ordered alloys is attractive because of the additional information available from the X-ray pattern.

Period for this MRP

1 - 65 to 12 - 65

MO YR MO YR

Sub-group

SIGNATURE OF  
PRINCIPAL  
INVESTIGATOR

Identify the Professional School (medical, dental, public health, graduate, or other) with which the project should be identified.

SCHOOL

Contractor: Michigan, University of, Ann Arbor, Michigan

Contract Number: AT(11-1)-1086

Present Contract Term: October 1, 1963 through September 30, 1964

Cost to AEC: \$31,397

Contract Title: THE OXIDATION OF SINGLE CRYSTAL FOILS

Investigators: Lawrence O. Brockway

Scope of Work:

Single crystal films of copper of 700A thickness prepared by condensation onto NaCl substrates have been subjected to annealing treatments which produce either (a) dislocation densities of about  $10^9 \text{ cm}^{-2}$  and almost no stacking faults, or (b) dislocation densities of about  $10^7 \text{ cm}^{-2}$ , wide stacking faults with areas of  $5 \times 10^4 \text{ cm}^2$  per  $\text{cm}^3$  of film, and terraces on the surface with heights of 50 to 300 A.

Treatment of the films with oxygen at  $525^\circ\text{C}$  and  $0.9 \mu$  pressure produces two epitaxial orientations of  $\text{Cu}_2\text{O}$  with (111) or (001) parallel to the  $\text{Cu}(001)$ . The smallest oxide grains are  $0.2 \mu$  after 2 minutes and reach  $1.0 \mu$  after 15 minutes. On the films having stacking faults the oxide nuclei tend to lie on or near the faults; many of the grains grow preferentially along the faults. On the films without faults the density of oxide nucleation sites is usually greater than on the films with faults.

Condensed nickel films annealed on NaCl also show wide stacking faults without the high concentration of twins found in the unannealed films.

Further work includes (a) use of other alkali halide substrates for Cu and Ni in a test of the substrate influence on stacking fault formation; (b) oxidation of Cu and Ni films in a gas reaction chamber in an electron microscope allowing continuous observation during the oxidation; (c) the effect of strains due to stretching and bending of the films, to the presence of foreign atoms, and to the occurrence of grain boundaries in thinned polycrystalline films.

Recent Publications:

L. O. Brockway and R. B. Marcus, "Microstructure of Thin Single Crystals of Copper," J. Appl. Phys. 34, (1963) p. 921

R. B. Marcus and L. O. Brockway, "Oxidation of Thin Single Crystals of Copper," Inorg. Chem. 2, (1963) p. 489

Contractor: Michigan, University of, Ann Arbor, Michigan  
Contract Number: AT(11-1)-1352  
Present Contract Term: December 1, 1963 through November 30, 1964  
Cost to AEC: \$115,000  
Contract Title: THERMODYNAMIC AND TRANSPORT PROPERTIES OF LIQUID METAL SYSTEMS  
Investigators: R. D. Pehlke

Scope of Work:

Phase I

The following areas of activity are being pursued:

- 1) a new program to determine the thermodynamic significance of the importance of oxygen, carbon and nitrogen in the corrosion of refractory metals in alkali metal environments;
- 2) a new program to ascertain the effect of dissolved oxygen on the activity coefficient of aluminum and uranium in bismuth base systems;
- 3) continuation of a study originated during the preceding period involving the experimental determination of the importance of the dimerization reaction in alkali metal vapors on the thermal conductivity;
- 4) continuation of the optical absorption program for obtaining thermodynamic data.

Phase II

This project is concerned with measuring the electric mobility of solute atoms in liquid metals. Accurate measurements of mobility are being made in the system Bi-Sn as a function of temperature and composition. Attempts are being made to correlate the mobility measurements with thermodynamic properties. Diffusion potential measurements are being attempted for use with the mobility data to verify the Onsager reciprocity relations.

### Phase III

This project is directed at measuring interactions between solutes in dilute solution, and correlating these data for use in predicting activities of solutes in multi-component metal systems.

Atomic interaction in dilute molten alloys has been studied in several systems utilizing the electromotive force technique. The proposed research would extend these measurements to other systems, and to multi-component alloys. The systems proposed for study include the influence of several alloying elements on the activity of zinc in liquid bismuth, on the activity of uranium in liquid bismuth, and the activity of zinc in liquid lead. It is proposed to extend these studies to multi-component solution to evaluate various correlations for predicting the activity of a component in a complex alloy. The interaction between hydrogen and dissolved solutes in liquid nickel is also proposed for study. Correlation of the investigations of atomic interaction in metallic solutions would involve correlations of experimental results with physical properties, i.e., magnetic susceptibility, number of free electrons, valency, electromotive force, and other properties which can be determined independent of the thermodynamic measurements.

**Contract:** University of Minnesota, Minneapolis, Minnesota

**Contract Number:** AT(11-1)-532

**Present Contract Term:** June 1, 1964 through September 30, 1964

**Cost to AEC:** \$12,890

**Contract Title:** EFFECT OF ATOMIC RADIATION AND OF MOLECULAR ORIENTATION ON MECHANICAL BEHAVIOR OF LINEAR HIGH POLYMERS

**Investigators:** C. C. Hsiao

**Scope of Work:**

Certain aspects of research concerning the effect of molecular orientation on the anisotropic behavior of oriented linear high polymers will be studied and completed. Both analytical and experimental investigations on dynamic mechanical properties of polymers of various degrees of anisotropy will be reported. Using plane wave propagation technique, uniaxial strength and fracture of a series of oriented polymer rods will be obtained.

It is also hoped to learn some additional knowledge on the internal strength and fracture characteristics by using the recent novel accomplishment in reflecting and focusing compressive pulses in three dimensions. Spheroidal specimens of different sizes will be used. An attempt will be made to analyze the internal stresses and fracture created by the reflected tensile pulse. The fracture strength will be correlated with the state of stress. Other relevant studies such as time dependent viscoelastic behavior of transversely isotropic polymers will also be carried out.

**Recent Publications:**

C. C. Hsiao and T. S. Wu, "Analysis of Orientation and Strength of Branched Polymer Model Solid," J. Polymer Science, Part A, Vol. 1, pp. 1789-1797, (1963)

C. C. Hsiao, "Time Dependent Fracture," Proceedings, Symposium on Structural Dynamics under High Impulse Loading, Technical Documentary Report No. ASD-TDR-63-140, (1963)

S. R. Moghe and C. C. Hsiao, "Stress Analysis of Nonhomogeneous Anisotropic Viscoelastic Cylinder," T. R. No. 19, AEC AT(11-1)-532, University of Minnesota, pp. 1-80, (1963); "Stress Analysis of Anisotropic Viscoelastic Hollow Cylinder," in press, to appear in the Proceedings of the Fourth International Congress on Rheology, (Brown University, 1963)

C. C. Hsiao and S. R. Moghe, "Stress Field and Fracturing of Solid Propellant during Rocket Firing," J. AIAA, Vol. 1, No. 8, pp. 1931-1932, (1963)

C. C. Hsiao and S. R. Moghe, "Viscoelasticity and Viscoelastic Stress Analysis," T. R. No. 20, AEC AT(11-1)-532, University of Minnesota, (1963)

S. R. Moghe and C. C. Hsiao, "Stress Distribution in Anisotropic Viscoelastic Hollow Sphere," T. R. No. 21, AEC AT(11-1)-532, University of Minnesota, (1963)

S. R. Kao and C. C. Hsiao, "Anisotropy of Oriented Materials," T. R. No. 22, AEC AT(11-1)-532, University of Minnesota, (1963)

C. C. Hsiao, "Molecular Orientation Dependent Fracture Strength," T. R. No. 23, AEC AT(11-1)-532, University of Minnesota, (1963); In press, to appear as a section of a book entitled "Fracture of Polymeric Solids," Interscience Publishers (John Wiley), New York

Contractor: Minnesota, University of, Minneapolis, Minnesota

Contract Number: AT(11-1)-841

Present Contract Term: November 1, 1963 through October 31, 1964

Cost to AEC: \$36,526

Contract Title: DIFFUSION STUDIES IN LIQUID METALS

Investigators: Richard A. Swalin

Scope of Work:

The diffusion of trace amounts of ruthenium, silver, indium, tin and antimony in liquid silver is being investigated as a function of temperature. These elements have valences relative to silver of -1, 0, +2, +3, and +4 respectively. If the coulombic term due to the valence difference makes a major contribution to the interaction of solutes and solvent one may then estimate the energetics of the solute-solvent interactions and hence obtain the relation of these energetics to the diffusivity of solutes. At present measurements for silver and tin have been completed. Work on cadmium is almost complete.

In addition, measurements will be made of the self-diffusivity and electrical resistivity of liquid sodium and potassium as a function of temperature under conditions of constant volume and constant pressure. By investigating the temperature dependence of these measurements, information concerning the role of density fluctuations in both atom transport and electron scattering may be obtained. Suitable high pressure apparatus is being constructed for these measurements.

Recent Publications:

C. H. Ma and R. A. Swalin, "Self-Diffusion in Liquid Tin," J. of Chemical Physics, Vol. 36, No. 11 (1962) pp. 3014-3018.

**Contractor:** Minnesota, University of, Minneapolis, Minnesota

**Contract Number:** AT(11-1)-1009

**Present Contract Term:** March 16, 1964 through March 15, 1965

**Cost to AEC:** \$15,618

**Contract Title:** A STUDY OF THE ANOMALOUS RESISTIVITY CHANGE ACCOMPANYING PLASTIC DEFORMATION IN CU-PD AND AG-PD ALLOYS

**Investigators:** Morris E. Nicholson

**Scope of Work:**

In certain alloy systems, such as Au-Pd, Ag-Pd and Cu-Pd, the electrical resistivity initially decreases when some of the alloys are deformed plastically. This behaviour is abnormal. In most pure metals and alloys the electrical resistivity increases when the alloys are plastically deformed because the deformation process produces lattice defects which scatter electrons thus increasing resistivity. This research is directed at determining the cause of this unusual effect.

Research to date has shown the number of conduction electrons increases with plastic deformation, that this is caused by a destruction of short range order and that the resistivity increases with low temperature annealing in a way indicating the annealing permits diffusion primarily of vacancies to re-establish short range order.

A study is continuing on the influence of plastic deformation on the destruction of short range order in Au-Pd alloys, the influence of strain hardening on mobility of electrons.

**Contractor:** Mississippi, University of, University, Mississippi

**Contract Number:** AT(40-1)-2891

**Present Contract Term:** September 15, 1963 through September 14, 1964

**Cost to AEC:** \$41,427

**Contract Title:** THE EFFECTS OF NEUTRON IRRADIATION ON THE ELECTRONIC PROPERTIES OF BINARY ALLOYS

**Investigators:** Arthur B. Lewis

**Scope of Work:**

Employing a 3 mev accelerator to produce fast neutrons, the Department of Physics and Astronomy at the University of Mississippi will irradiate binary alloys at various compositions and at various temperatures lying on both sides of the phase boundary. Resistivity measurements will be made on the irradiated samples before and after heat treatments and irradiations. An attempt will also be made to determine if Cu, 15%Al alloys annealed at around 300°C to room temperature will suffer a large change in resistivity upon being irradiated with fast neutrons. The range of temperature from 75° K to 700° K will be explored. The neutron source will be essentially free of thermal neutrons; generally, 14 mev neutrons from the D,T-n reaction will be used to irradiate the alloy samples.

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SUPPORTING AGENCY: Atomic Energy Commission

TITLE OF PROJECT:

Grain Boundary Sliding in Alumina Bicrystals

Give names, departments, and official titles of PRINCIPAL INVESTIGATORS and ALL OTHER PROFESSIONAL PERSONNEL engaged on the project.

Dr. Hayne Palcoux III, Research Associate Professor, Department of Engineering Research

Mr. Paul M. Davis, Jr., Research Associate, Department of Engineering Research

\$29,944

NAME AND ADDRESS OF INSTITUTION:

North Carolina State of the University of North Carolina  
at Raleigh, Raleigh, N. C.

SUMMARY OF PROPOSED WORK - (200 words or less. Omit confidential data.) - In the Science Information Exchange summaries of work in progress are exchanged with government and private agencies supporting research, and are forwarded to investigators who request such information. Your summary is to be used for these purposes.

The object of the proposed work is to study grain boundary sliding in alumina bicrystals with both clean and doped grain boundaries. The mechanism by which grain boundary sliding occurs should change as the nature of the grain boundary changes from no impurity to a glassy phase impurity, to a crystalline phase impurity (including both reaction phases such as  $MgAl_2O_4$  and non-reactive phases such as a noble metal). The alumina bicrystals are formed by a pressure sintering technique, allowing precise control to be exercised over the orientation of the adjacent crystals and the impurity and concentration in the grain boundary. Initially, the research program will be concerned with the effects of orientation of adjacent crystal halves, test temperature, and strain rate on the grain boundary sliding behavior of clean, undoped bicrystals. The second phase of the research program will be directed toward determining the effects of controlled additions of impurities to the grain boundary.

Period for this NRP			
_____ to _____		_____	
MO	YR	MO	YR
Sub-group			

SIGNATURE OF PRINCIPAL INVESTIGATOR \_\_\_\_\_

Identify the Professional School (medical, dental, public health, graduate, or other) with which this project should be identified:

SCHOOL \_\_\_\_\_

INVESTIGATOR -- DO NOT USE THIS SPACE

**Contract:** Missouri, University of, Rolla, Missouri  
(School of Mines and Metallurgy)

**Contract Number:** AT(11-1)-1368

**Present Contract Term:** May 1, 1964 through April 30, 1965

**Cost to AEC:** \$47,732

**Contract Title:** FERROELECTRIC PROPERTIES OF BISMUTH FERRATE AND  
RELATED MATERIALS

**Investigators:** Robert Gerson

**Scope of Work:**

The properties of the perovskite, bismuth ferrate, and solid solutions of this material with other perovskites and related ferroelectrics, are to be investigated. Bismuth ferrate has a rhombohedral (perovskite) crystalline structure with a reported rhombohedral angle of  $89^{\circ}25'$ . This deviation from cubic symmetry is almost twice that of any known rhombohedral perovskite ferroelectric. Indirect evidence has been advanced that bismuth ferrate is ferroelectric and has a very high ferroelectric Curie point,  $850^{\circ}\text{C}$ , coinciding with the temperature at which it undergoes incongruent fusion. Neutron diffraction studies have also shown that bismuth ferrate is anti-ferromagnetic, with a Neel temperature close to  $400^{\circ}\text{C}$ .

The primary purpose of this research will be the investigation of bismuth ferrate itself with a view to clarifying its dielectric properties. Solid solutions of bismuth ferrate, including those with lead zirconate and lead zirconate-lead titanate, will be prepared and the dielectric, ferroelectric, and piezoelectric properties determined. An attempt will be made to prepare bismuth scandate, a possible isomorph of bismuth ferrate, which may have a lower conductivity and, consequently, ferroelectric properties which can be more easily observed.

**Contract:** National Bureau of Standards, Washington, D.C.

**Contract Number:** NBS Project No. 09450

**Present Contract Term:** October 1, 1963 through September 30, 1964

**Cost to AEC:** \$65,000

**Contract Title:** HIGH TEMPERATURE CRYSTAL GROWTH TECHNIQUES

**Investigators:** W. S. Brower

**Scope of Work:**

The objective of this program is the development of techniques for high temperature crystal growth from melts with the best possible control of purity, defects, and orientation.

The plasma torch has been used to grow small crystals of  $ZrO_2$  stabilized by CaO to gain knowledge which will be used to proceed on to more refractory crystals melting near  $3000^\circ C$ .

The direct electromagnetic method of heating for floating zone crystal growth has progressed to the point where molten zones have been moved through polycrystalline NiO and  $MnFe_2O_4$ . Attempts will be made to extend this technique to higher resistivity materials such as  $Cr_2O_3$ . The ultimate objective is floating zone crystal growth of semiconductive materials.

Using electron microscopy, a precipitate phase, individual dislocations and stacking faults have been observed in  $TiO_2$  doped with 0.1% NiO.

**Contract:** National Bureau of Standards, Washington, D.C.

**Contract Number:** NBS Project No. 13443

**Present Contract Term:** October 1, 1963 through September 30, 1964

**Cost to AEC:** \$22,000

**Contract Title:** DIELECTRIC AND ELASTIC PROPERTIES OF CRYSTALS

**Investigators:** H.P.R. Frederikse and J. H. Wasilik

**Scope of Work:**

The research is a study of the lattice dynamics of pure and impure inorganic crystals by measuring the dielectric and elastic constants (real and imaginary parts) of these crystals.

The dielectric constant  $\epsilon$  of cubic  $\text{PbF}_2$  was measured from 1.9-300°K. is rather high ( $\epsilon = 28.4$  at room temperature) and increases  $\sim 15\%$  toward liquid helium temperatures. Simultaneous determination of the refractive index made it possible to evaluate the electronic polarizability  $[(4\pi/3) (\alpha_{el}/V) = .412]$  and the ionic contribution  $[(4\pi/3) (\alpha_{ion}/V) = .488]$ .

The elastic constants of  $\text{PbF}_2$  were measured at 300°K by means of a pulse echo technique. From these data a Debye temperature of 221.2°K was deduced. This work is now readied for publication.

Attempts to detect the contribution of excitons to the dielectric constant of CdS have not been successful so far. The reason is probably the low light intensity and hence small exciton density. Illumination with laser light might be the solution.

While the emphasis in the program previously has been on the dielectric losses due to imperfections and foreign ions, it is the intention now to focus the attention on the intrinsic lattice constants and their behavior at transition points. It is felt that the lattice dynamics, the relation between elasticity and polarizability and the changes of these constants when structural transitions take place, are of prime importance.

**Contract:** University of Nebraska, Lincoln, Nebraska

**Contract Number:** AT(11-1)-525

**Present Contract Term:** June 1, 1964 through May 31, 1965

**Cost to AEC:** \$65,950

**Contract Title:** STUDIES OF IMPERFECTIONS IN SOLIDS

**Investigators:** Edgar A. Pearlstein

**Scope of Work:**

A. Radiation Effects in Metals

Copper foils are irradiated at liquid nitrogen temperature with protons and helium ions of energy 50 to 350 keV, and changes in electrical conductivity measured. The objective is to provide data with which to test the theory of radiation damage insofar as it predicts dependence upon energy and mass of the bombarding particles. Also, the possibility of surface effects is being studied by irradiating with low energy particles at oblique incidence.

Data have been obtained giving the dependence of radiation effects upon energy for protons and helium ions. In the case of helium ions, there is an inflection point, in the graph of resistivity change vs. energy, at an energy corresponding to the velocity at which  $\text{He}^+$  might be expected to become  $\text{He}^{++}$ .

There appears to be no surface effect for the conditions of these experiments.

B. Mechanisms for Color Center Production in Alkali Halides

Experimental work is being done on the following: (1) Interaction between growth rate of color centers and bleaching. (2) Dependence of colorability upon impurities. (3) Stored energy in x-rayed crystals. (4) Color centers and dislocations.

(1) It is found that, in some specimens of KCl and NaCl, simultaneous irradiation with x-rays and light predisposes the crystals to color considerably faster, on subsequent irradiation with x-rays in the dark, than if they had been originally irradiated in the dark.

(2) At  $0^\circ\text{C}$  the rate of coloration by x-rays is roughly proportional to the one-fifth power of the concentration of divalent cation impurities. At liquid nitrogen temperature, the rate is almost independent of the impurities.

(3) Crystals are irradiated with x rays at liquid nitrogen temperature. The heat given off as they are warmed to  $400^{\circ}\text{C}$  is measured and correlated with optical absorption. There are no data yet.

(4) Thin platelets of NaCl are grown from solution, and the positions of dislocations determined by an x ray technique. After irradiation with x rays, the platelets are scanned optically to see if there is a correlation between F-band absorption and dislocations. Results so far are scattered and inconclusive.

#### C. Point Defect Concentrations in Sodium Metal

Simultaneous measurements of x ray lattice parameter and length have been made on single crystals of sodium, over a temperature range from  $-26^{\circ}\text{C}$  to  $+96^{\circ}\text{C}$ , in order to obtain values for the net vacancy concentration at the melting point and for the energy of formation of vacancies. For two specimens, the results are: concentration of vacancies at the melting point  $\Delta N/N = 0.93 \times 10^{-3}$  respectively, and formation energy  $E_f = 0.13 \text{ eV}$  and  $0.12 \text{ eV}$  respectively.

#### D. Electron-Phonon Interaction Studies By Thermal Diffuse X-Ray Scattering

The influence of electron-phonon interactions on phonon spectra in metals is being studied by measuring the thermal diffuse x-ray scattering of metal crystals. Present work is directed toward determining whether the possible existence of Overhauser spin density waves in the electron gas of anti-ferromagnetic chromium can be detected through electron-phonon effects on the thermal diffuse x-ray scattering of chromium below and above its Néel temperature.

The image of the Fermi surface due to electron-phonon interactions (Kohn effect) will be studied in tin crystals.

#### Recent Publications:

Edgar Pearlstein, "Dynamical Theory of Atom Jumps in Crystals", Am. J. Phys. 31, 842 (1963).

Charles Skov and Edgar Pearlstein, "Nonlinear Ionic Conduction in Alkali Halide Crystals", BAPS 8, 268 (1963).

George A. Sullivan and John W. Weymouth, "Concentration of Point Defects in Sodium Metal", BAPS 9, 110 (1964).

Contractor: New York University, University Heights, New York

Contract Number: AT(30-1)-2916

Present Contract Term: January 1, 1964 through December 31, 1964

Cost to AEC: \$36,065

Contract Title: THERMODYNAMIC PROPERTIES OF INTERMETALLIC COMPOUNDS

Investigators: Kurt L. Komarek

Scope of Work:

The objective of the investigation is to obtain precise liquidus data for the homologous series Mg-Pb, Mg-Sn, Mg-Ge, and Mg-Si to permit a thermodynamic analysis of these systems, and to obtain electrical resistivities of the molten alloys. Deflections in the activity-concentration curves will be correlated with deflections in the resistivity-concentration curves and the trend of these deflections with the change in bonding character investigated.

The liquidus curves of the Mg-Sn and Mg-Pb system were accurately determined. A set of equations were derived which allows an accurate determination of the thermodynamic properties of liquid Mg-Sn alloys from liquidus data and enthalpies of mixing. The activity of magnesium shows a negative deviation from ideality, but the activity of tin both a negative and a positive deviation. The excess entropy of mixing is negative over the entire concentration range. It was found that  $Mg_2Pb$  transforms to a high temperature structure which has a maximum melting point of  $546.8^{\circ}C$  at 35.3 at. % Pb. The temperature-dependence of the lattice parameter of  $Mg_2Pb$  was determined by high-temperature x-ray diffraction. There is evidence of the existence of another compound, probably MgPb, stable over a narrow temperature interval.

**Contract:** University of North Carolina, Chapel Hill, North Carolina

**Contract Number:** AT(40-1)-2036

**Present Contract Term:** April 1, 1964 through March 31, 1965

**Cost to AEC:** \$19,098

**Contract Title:** RESEARCH IN INTERMETALLIC DIFFUSION

**Investigators:** Lawrence Slifkin

**Scope of Work:**

Four experiments aimed at increased understanding of point defects in crystals are to be performed. (a) The effect of a flux of vacancies on tracer diffusion will be measured in alloys of silver-gold. Vacancy fluxes will be established by means of chemical concentration gradients, and the tracer will consist of a thin layer of Au<sup>198</sup> originally placed at the sandwich interface. The success of the experiment hangs on the near-independence of the diffusion coefficient of Au over a large range of composition in Ag-Au alloys. (b) In an attempt to understand the atom movements involved in Zener stress-induced ordering anelasticity, comparison of activation energies of this process with those from tracer diffusion will be made. The diffusion of Ag and Cd in silver plus 30 and 38 atomic percent cadmium will be compared with internal friction data of Turner and Williams of Wake Forest College. (c) A "geometrical" model of the effect of ordering on tracer diffusion attributes the decrease in diffusion upon ordering to the necessity for producing anti-order when vacancies move. Further understanding of the processes involved will be sought from experiments on self-diffusion in Cu<sub>3</sub>Au, where it is expected that the decrease in mobility of the Au will be enormously greater than that of Cu. (d) Earlier experiments on quenched AgCl indicate the presence of divacancy pairs. These will be examined by dielectric relaxation. Moreover, the effect of x-irradiation on the annealing-out of these pairs will be further studied in an attempt to untangle the processes involved.

**Recent Publications:**

Kabler, et al., "Point-Defects and Dislocations in AgCl," Materials Science Research, Vol. 1 (N.Y. Plenum Press, 1963).

Williams and Slifkin, "Anomalous Diffusion of Rare Earth Tracers in Ag and Pb," Acta Met., 11, (1963) p. 319.

Mallard, et al, "Self-Diffusion in Ag-Au," Phys. Rev. 129, (1963) p. 617.

**Contract:** University of North Carolina, Chapel Hill, North Carolina

**Contract Number:** AT(40-1)-2577

**Present Contract Term:** June 1, 1964 through May 31, 1964

**Cost to AEC:** \$32,980

**Contract Title:** RADIATION DAMAGE AND OTHER STUDIES BY MEANS OF A VAN DE GRAAFF ACCELERATOR

**Investigators:** Paul E. Shearin

**Scope of Work:**

Radiation damage studies in gold, aluminum, and alloys of aluminum are underway. Damage is introduced through electron bombardment at temperatures near  $10^{\circ}\text{K}$ ,  $21\text{ K}$ , and  $78^{\circ}\text{K}$ , the damage being measured through change in electrical resistance. Threshold for damage is determined and recovery of damage is studied through isochronal anneals for temperatures up to  $300^{\circ}\text{K}$ . Radiation anneals are also studied.

Nuclear energy levels are studied through Coulomb Excitation by proton bombardment and subsequent measurements of the de-excitation gamma rays. Energy levels in light nuclei having nuclear reactions of low  $Q$  values are studied by deuteron stripping processes.

SCIENCE INFORMATION EXCHANGE  
SMITHSONIAN INSTITUTION

NOT FOR PUBLICATION OR  
PUBLIC CITED REFERENCE

PROJECT NO. (Do not use this space)

SUPPORTING AGENCY: Atomic Energy Commission

TITLE OF PROJECT:

Grain Boundary Sliding in Alumina Bicrystals

Give names, departments, and official titles of PRINCIPAL INVESTIGATORS and ALL OTHER PROFESSIONAL PERSONNEL engaged on the project.

Dr. Hayne Palcoux III, Research Associate Professor, Department of Engineering Research

Mr. Paul M. Davis, Jr., Research Associate, Department of Engineering Research

\$29,944

NAME AND ADDRESS OF INSTITUTION:

North Carolina State of the University of North Carolina

at Raleigh, Raleigh, N. C.

SUMMARY OF PROPOSED WORK - (200 words or less. Omit confidential data.) - In the Science Information Exchange summaries of work in progress are exchanged with government and private agencies supporting research, and are forwarded to investigators who request such information. Your summary is to be used for these purposes.

The object of the proposed work is to study grain boundary sliding in alumina bicrystals with both clean and doped grain boundaries. The mechanism by which grain boundary sliding occurs should change as the nature of the grain boundary changes from no impurity, to a glassy phase impurity, to a crystalline phase impurity (including both reaction phases such as  $\text{MgAl}_2\text{O}_4$  and non-reactive phases such as a noble metal). The alumina bicrystals are formed by a pressure sintering technique, allowing precise control to be exercised over the orientation of the adjacent crystals and the impurity and concentration in the grain boundary. Initially, the research program will be concerned with the effects of orientation of adjacent crystal halves, test temperature, and strain rate on the grain boundary sliding behavior of clean, undoped bicrystals. The second phase of the research program will be directed toward determining the effects of controlled additions of impurities to the grain boundary.

Period for this NRP		SIGNATURE OF PRINCIPAL INVESTIGATOR
____ to ____ mo yr mo yr		
Sub-group		Identify the Professional School (medical, dental, public health, graduate, or other) with which this project should be identified:
		SCHOOL

INVESTIGATOR — DO NOT USE THIS SPACE

Contractor: North Dakota, University of, Grand Forks, North Dakota

Contract Number: AT(11-1)-1255

Present Contract Term: June 1, 1964 through May 31, 1965

Cost to AEC: \$11,329

Contract Title: RADIATION DAMAGE TO SILICA STRUCTURES

Investigators: Harold D. Bale

Scope of Work:

Our present work is concerned with the study of the changes that occur in the structure of silica gels upon pile irradiation. Structural changes related to the size range of the gel are being studied by small angle x-ray scattering while changes in the arrangement of the atoms in the solid are being studied by large angle x-ray diffraction. Results of our study indicate that both types of structural changes occur upon irradiation.

The surface area of all the silica gels studied were reduced after an irradiation dose of  $5 \times 10^{19}$  fast neutrons. The effects are most pronounced for the higher area samples. These changes in surface appear to be stable over a period of six months and cannot be removed by heat treatment. Initial large angle diffraction studies indicate that  $\text{SiO}_4$  tetrahedra in the gel are altered by irradiation in the same fashion as in vitreous silica.

Future study will consider the irradiation effects as a function of total flux to see if saturation of the damage occurs. Also the effects of high temperature, gamma radiation and x-rays on the gels will be examined.

**Contract:** Northwestern University, Evanston, Illinois

**Contract Number:** AT(11-1)-1053

**Present Contract Term:** June 15, 1964 through June 15, 1965

**Cost to AEC:** \$77,256

**Contract Title:** RADIATION EFFECTS OF POSITIVE ION BOMBARDMENT

**Investigators:** R. L. Hines

**Scope of Work:**

The objective of this work is to investigate the damage formed in single crystal gold foils by ion bombardment with ion energies between 5 and 50 kev using transmission electron microscopy to observe the imperfections created by the bombardment. This investigation should confirm the suspected one to one correspondence between the impact of a single positive ion and the formation of an imperfection cluster in the foil which can be observed with an electron microscope. By varying the ion energy and mass it should be possible to determine the minimum conditions for the formation of an observable imperfection cluster. The gold foils will be formed by vacuum evaporation of gold on to a hot, freshly-cleaved rock salt substrate. After dissolving the rock salt with water and mounting the foils on electron microscope grids, they will be bombarded by mass analyzed ion beams at energies between 5 and 50 kev. After bombardment the foils will be transferred to the electron microscope for examination by transmission. The ion bombardment equipment is in operation, gold foils with thicknesses between 250A and 500A have been prepared, and preliminary investigations show that the foils have good single crystal diffraction patterns.

Contractor: Northwestern University, Evanston, Illinois

Contract Number: AT(11-1)-1126

Present Contract Term: February 1, 1964 through January 31, 1965

Cost to AEC:

Contract Title: CONTRIBUTION TO THE UNDERSTANDING OF THE HIGH TEMPERATURE OXIDATION OF METALS

Investigators: J. Bruce Wagner, Jr.

Scope of Work:

Oxidation studies on iron in CO-CO<sub>2</sub> mixtures [F. Pettit, R. Yinger & J. B. Wagner, Jr., "The Mechanism of Oxidation of Iron in CO-CO<sub>2</sub> Mixtures," *Acta Met.* 8 (1960); F. Pettit and J. B. Wagner, Jr., "Transition from Linear to Parabolic Kinetics During the Oxidation of Iron in CO-CO<sub>2</sub> Mixtures," *Acta Met.*, (in Press)], and cobalt [F. Pettit and J. B. Wagner, Jr., *Acta Met.*, (in Press)] have shown that at high temperatures a thick compact layer of wüstite forms and the rate determining step is the dissociation of CO<sub>2</sub> into CO and absorbed oxygen according to an equation due to C. Wagner,  $\dot{R}/A = k'P(1 + K) [N'_{CO_2}(eq)]$

where  $\dot{R}$  is the number of equivalent of oxides per second, A the sample area, k' the rate constant of phase boundary reaction, P the sum of the partial pressures of CO and CO<sub>2</sub>, K the equilibrium constant of CO, CO<sub>2</sub> iron and wüstite, N'<sub>CO<sub>2</sub></sub> the mole fraction of CO<sub>2</sub> in the oxidizing gas and N<sub>CO<sub>2</sub></sub>(eq) the mole fraction of CO<sub>2</sub> in the oxidizing gas and N'<sub>CO<sub>2</sub></sub>(eq) the mole fraction of CO of CO<sub>2</sub> coexisting with Fe/FeO.

Alloys containing small amounts of chromium in iron and of titanium in iron exhibit slower linear kinetics than does the pure iron. Both the alloying agents enter wüstite under the formation of additional cation vacancies and a decreased concentration of electron holes. The present study is aimed at determining why an increase in vacancy concentration coincides with decreased linear kinetics.

The bulk properties of undoped wüstite doped with chromium or titanium have been studied using electronic conductivity, lattice parameter measurements and thermoelectric effect measurements. Results confirm the increased vacancy concentration with increasing oxygen concentration and with additions of Cr or Ti under fixed oxygen pressures. In addition a p-n transition in wüstite is observed at high oxygen concentrations and at high temperatures. The present work will include a thermogravimetric study on these materials to aid in understanding the transport properties.

Recent Publications:

F. Pettit and J. B. Wagner, Jr., "Transition from the Linear to the Parabolic Rate Law During the Oxidation of Iron to Wüstite in CO-CO<sub>2</sub> Mixtures," Accepted by Acta Met.

F. Pettit and J. B. Wagner, Jr., "Studies on the Oxidation of Cobalt," Accepted by Acta Met.

**Contract:** Northwestern University, Evanston, Illinois

**Contract Number:** AT(11-1)-1161

**Present Contract Term:** April 1, 1964 through March 31, 1965

**Cost to AEC:** \$38,000

**Contract Title:** STUDY OF RADIATION DAMAGE RESULTING FROM ELECTRON BOMBARDMENT

**Investigators:** John W. Kauffman

**Scope of Work:**

This research is directed toward the determination of the nature and detailed mechanisms of the interactions between incident energetic electrons and the lattice of crystalline materials. Both the dynamics of "damage" production and the nature and properties of the resulting lattice imperfections are of interest. A large number of the physical properties of materials are affected by electron irradiation to varying degrees, and, therefore, the dual closely related objectives of the use of irradiation as an approach to better understanding of the general properties of materials such as, for example, atomic diffusion as well as the determination of the fundamental nature of radiation damage itself is apparent. At the present state of development of this field, our work is directed primarily toward the basic nature of the lattice defects and dynamics of production. Certain physical properties are presently chosen for investigation on the basis of closeness and directness in relation to the fundamental imperfections and processes. Electrical resistivity determined at liquid helium temperatures is most often used and correlated with other physical properties.

A new additional Van de Graaff laboratory has been recently set up by this University for irradiation studies of materials and is now in operation. Associated low temperature cryostats and measuring equipment are in operation.

Recent published research involve the nature of Stage I recovery in pure copper; new substages have been discovered and further studies are in progress involving the detailed kinetics with the objective of determining the precise atomic processes involved in the various substages. It was observed that similarities with the previously studied recovery spectrum of gold indicate that the same type of interstitial occurs for both metals, but the distribution of close pairs and strength of interactions forming clusters appears to be markedly different for these two metals.

**Recent Publications:**

John A. Tesk, E. C. Jones, Jr., and J. W. Kauffman, "Stage I Recovery Spectrum of Pure Copper Irradiated with Electrons over the Range 1.25 to 3.25 MeV," Physical Review, Vol. 133, No. 1A, (1963) pp. A288-A293.

Contract: Northwestern University, Evanston, Illinois

Contract Number: AT(11-1)-1367

Present Contract Term: April 1, 1964 through March 31, 1965

Cost to AEC: \$21,723

Contract Title: EFFECT OF POINT DEFECTS ON MECHANICAL PROPERTIES  
OF METALS

Investigators: M. Meshii

Scope of Work:

The purpose of the present project is to investigate the effect of point defects on the mechanical behavior of metallic single crystals with special emphasis placed on the point defects produced by particle irradiation. Electron irradiation is chosen here, since it can produce the simplest damage by choosing a suitable beam energy and past information on the structure after irradiation is most readily available for comparison.

A cryostat in which the electron irradiation and a mechanical test can be performed without transfer at temperatures ranging from 5° to 300°K will be used. The effect of the irradiation on flow stress, work-hardening coefficient and general shape of stress-strain relation (yield drop and extents of Stages I, II, and III of deformation) will be studied by varying: (1) the dosage, (2) energy of the electron beam, (3) the temperature of irradiation, and (4) the possible annealing following the irradiation. The relation between the effect of the electron irradiation and the initial structure of the specimens (the impurity contents, the concentration of vacancies and the density of dislocations prior to the irradiation) will also be studied. Aluminum will be first used for specimen material, and further work will include other face-centered-cubic metals and metals of other crystal structures.

It is expected that the present study will provide fundamental information in radiation-hardening as well as resulting in further understanding the role of point defects in strength of metals.

### An Investigation of Mixed Conduction in Solid Electrolytes

(Give names, departments, and official titles of PRINCIPAL INVESTIGATORS and ALL OTHER PROFESSIONAL PERSONNEL engaged on the project.)

**Robert A. Rapp, Assistant Professor**  
Department of Metallurgical Engineering  
The Ohio State University

NAME AND ADDRESS OF INSTITUTION:

\$27,100

**The Ohio State University, 124 West 17th Avenue, Columbus, Ohio 43210**

**SUMMARY OF PROPOSED WORK** -- (Approximately 200 words. Omit confidential data.) In the Science Information Exchange summaries of work in progress are exchanged with government and private agencies supporting research, and are forwarded to investigators who request such information. Your summary is to be used for these purposes. Please make your summary substantive in nature, rather than generally descriptive.

The proposed research includes four specific types of experimental investigations:

(a) From A.C. conductivity measurements as a function of oxygen chemical potential, determine the ionic and electronic partial conductivities in cubic solid solutions of  $ZrO_2$  doped with various concentrations of  $CaO$ . A specification of the particular interactions in these solid solutions between the  $Ca$  cations, the anion vacancies, and conduction electrons is the purpose of this part of the research.

(b) From analogous A.C. experiments and from D.C. polarization measurements on  $ThO_2$  doped with various concentrations of  $Y_2O_3$  and rare earth oxides of the general formula  $(M_2O_3)$ , determine the oxygen potential at which significant electronic conductivity appears. The purpose of this part of the research is to determine the optimum binary oxide system and composition, and its limiting oxygen potentials.

(c) Using the galvanic cell technique involving a solid electrolyte suitable for very low oxygen pressures, (probably  $ThO_2+Y_2O_3$ ) determine the absolute and relative stabilities of the four modifications of the compound  $SiO_2$  (cristobalite, tridymite, high quartz, and vitreous quartz). Solid electrolyte galvanic cell determinations of the stabilities of other oxides (e.g.  $Cr_2O_3$ ,  $MnO$ ,  $NbO$ , etc.) may be attempted.

(d) From the dependence on nitrogen pressure of the total conductivity of pure and doped ionic nitrides, ( $Th_3N_4$ ,  $Be_3N_2$ ,  $Mg_3N_2$ , and  $AlN$ ) determine the partial ionic and electronic conductivities in these nitrides, gain some knowledge concerning the conduction mechanisms, and evaluate the possibility of finding or designing a solid nitride electrolyte for galvanic cells.

Period for this NRP			
_____ to _____			
MO	YR	MO	YR
Sub-group			

SIGNATURE OF PRINCIPAL INVESTIGATOR \_\_\_\_\_

Identify the Professional School (medical, dental, public health, graduate, or other) with which this project should be identified:  
SCHOOL **Engineering (graduate)**

Contract: Notre Dame, University of, Notre Dame, Indiana

Contract Number: AT(11-1)-1375

Present Contract Term: May 1, 1964 through April 30, 1965

Cost to AEC: \$13,000

Contract Title: MAGNETOELASTIC PHENOMENA IN METALS

Investigators: B. D. Cullity

Scope of Work:

The proposed research is concerned with stress-induced magnetic anisotropy in ferromagnetic materials, chiefly nickel. Uniaxial plastic elongation of a few percent has been found to produce residual stresses which cause X-ray diffraction line shifts and changes in magnetostriction. The latter indicate that domain vectors in most of the volume of the nickel specimen are aligned parallel to the axis of previous elongation, so that this axis becomes one of relatively easy magnetization.

This anisotropy will be investigated directly, by measurements with a torque magnetometer, and indirectly, by analysis of magnetization curves. Particular attention will be paid to the region of deformation below 5 percent elongation. Where necessary, residual stresses will be measured by means of X-ray diffraction.

Further measurements of magnetostriction will be made, and these may be complemented by magneto-resistance measurements. The possibility of developing a magnetic method of measuring residual stress will not be overlooked.

Contract: Oklahoma, University of, Norman, Oklahoma

Contract Number: AT(40-1)-2570

Present Contract Term: May 1, 1964 through April 1, 1965

Cost to AEC: \$16,006

Contract Title: INFLUENCE OF HYDROGEN ON MECHANICAL PROPERTIES OF METALS

Investigators: Raymond D. Daniels

Scope of Work:

The influence of hydrogen on the mechanical properties of columbium at low temperatures is under study. The effect of hydrogen contents below the limit of solubility on the ductile-brittle transition behavior is in columbium of special interest. The re-distribution of hydrogen within the metal lattice following pre-strain tensile testing at low temperatures.

The hydrogen sorption process in columbium is being studied as a function of temperature and grain size by measuring the rate of approach to equilibrium of columbium samples in an atmosphere of hydrogen.

Paul W. McDaniel, Director  
Division of Research

W. F. Shoely, Metallurgy and Materials  
Programs, Division of Research

NEW CONTRACT WITH UNIVERSITY OF OKLAHOMA (PLINT)

This is a research proposal aimed at three interrelated objectives:

- a) To obtain accurate values of the formation energies  $g_+$  and  $g_-$  for individual cation and anion vacancies in potassium chloride.
- b) To make a test of the theory of charged dislocations by two independent experiments.
- c) To obtain an improvement in the theory of charged dislocations by consideration of the effects of association of defects at low temperatures.

Professor Flint's thesis is that light scattering experiments and experiments which measure the temperature dependence of the voltage induced across crystals subject to deformation provide two independent methods of measuring  $(g_+ - g_-)$ , the difference between the formation energies of anion and cation vacancies in alkali halides. This, with ionic conductivity experiments which measure  $(g_+ - g_-)$ , provides sufficient information to determine the values of  $g_+$  and  $g_-$ .

Flint and Rezig have conducted research on light scattering from imperfection clouds around dislocations and recently published their results and their theory explaining the results in *J. Appl. Phys.*, Vol. 35, p. 2745 (1964). Essentially the proposal is a continuation of this research.

The proposal was reviewed by Grossweiner, IIT; Weigand, Carnegie; Crawford and Sander, ORNL; and Simpson and Tosi, AEL. The consensus of the first five is that the proposal is basically sound, of current interest and that Professor Flint is well qualified to conduct the program. Several people especially noted that Flint's unique approach should be fostered. Dr. Tosi of AEL wrote a detailed critique which I forwarded to Professor Flint for consideration. Tosi's remarks revealed to Flint an error he had made in his and Rezig's published theory. In his response to the reviewer's comments Flint concurred with Tosi's analysis and corrected the theory and showed that its application brought his experimental values for  $g_+$  and  $g_-$  in  $KCl$ ,  $KBr$ , and  $KI$  into closer agreement with Davidge, who approached the problem somewhat differently.

OFFICE ▶						
SURNAME ▶						
DATE ▶						

January 25, 1965

I believe that Flint's response to Toei's comments satisfactorily answer the criticisms and that the proposal should be accepted since results to be obtained are very fundamental to much of Metallurgy and Materials' solid state programs. The budget is as follows:

AEC Funds	\$17,262
University Contribution	<u>4,473</u>
TOTAL	\$21,735

Included in the AEC request are two items of capital equipment totalling \$1,225. The University plans to contribute \$1,500 in permanent facilities. I believe that this budget is satisfactory and that the proposal should be funded as requested, with title to the capital equipment vested in the contractor in consideration of his contribution.

OFFICE ▶						
SURNAME ▶						
DATE ▶						

**Contract:** Oregon State University, Corvallis, Oregon

**Contract Number:** AT(45-1)-1922

**Present Contract Term:** March 16, 1964 through March 15, 1965

**Cost to AEC:** \$32,367

**Contract Title:** THE ELECTRONIC PROPERTIES OF LIQUID SEMICONDUCTORS

**Investigators:** Melvin Cutler

**Scope of Work:**

The electronic structure of liquid semiconductors and their relation to liquid metals will be investigated, chiefly by measurements and analysis of electronic transport parameters: electrical and thermal conductivity, Hall coefficient and Seebeck coefficient. Attention will be centered on one or a few systems such as binary solutions of thallium and tellurium, which exhibit both semiconductor and metallic behavior at different temperatures and compositions. Experimental results will be analyzed in the light of transport theory, in a manner similar to what has been done with solids, in order to elucidate the electronic structure and scattering mechanisms which occur in the liquid state.

Contract: Pennsylvania State University, University Park,  
Pennsylvania

Contract Number: AT(30-1)-1710

Present Contract Term: April 1, 1964 through March 31, 1965

Cost to AEC: \$84,642

Contract Title: RESEARCH ON GRAPHITE

Investigators: W. S. Diethorn, P. L. Walker, Jr., and H. B. Palmer

Scope of Work:

I. Experiments will be commenced on the gasification kinetics of carbon films, using the techniques developed in studies of film formation kinetics.

II. Studies will continue on:

- A. The thermoelectric power of graphite as affected by gas chemisorption.
- B. Catalysis of the graphite-carbon dioxide reaction, examining catalysis by nickel and cobalt, again using magnetic susceptibility measurements to identify phases.
- C. The importance of active site area on the kinetics of the carbon-oxygen reaction.
- D. The electrical resistivity and thermoelectric power of boron-doped graphite.
- E. The physical structure of molecular sieve carbons.
- F. The use of tracer Xe to measure surface heterogeneity on carbons (technique may well show general applicability to other solid surfaces).
- G. Light microscope motion picture studies of graphite single crystal oxidation.
- H. The study of natural graphite with emphasis on radiation damage and thermal annealing.
- I. Natural graphite to include electron microscopy and the effects of oxidation and stress on Xe release.
- J. Xe release from petroleum cokes and other multicrystalline carbons specifically prepared for the program.

Recent Publications:

P. L. Walker, Jr. and B. C. Banerjee, "Topography of Kish Crystals and the Effect of Oxidation in Air," Nature, 197, (1963) p. 1291.

N. R. Laine, F. J. Vastola, and P. L. Walker, Jr., "The Importance of Active Surface Area in the Carbon-Oxygen Reaction," J. Phys. Chem., 67, (1963) p. 2030.

Recent Publications: continued

H. B. Palmer and T. J. Hirt, "The Activation Energy for the Pyrolysis of Methane," J. Phys. Chem., 67, (1963) p. 709.

T. J. Hirt and H. B. Palmer, "Kinetics of Deposition of Carbon Films from Methane and Carbon Suboxide," Carbon, 1, (1963) p. 65.

H. B. Palmer, "Carbon Deposition Kinetics in Isothermal Flow Systems," Carbon, 1, (1963) p. 55.

Contractor: Pennsylvania State University, University Park,  
Pennsylvania

Contract Number: AT(30-1)-1858

Present Contract Term: October 1, 1963 through September 30, 1964

Cost to AEC: \$20,200

Contract Title: EFFECT OF RADIATION ON DYNAMIC PROPERTIES OF HIGH  
POLYMERS

Investigators: A. E. Woodward

Scope of Work:

One phase of our studies concerned with the growth of single crystals of poly (4 methyl pentene-1) and examination of their properties and morphological features by x-ray and nuclear magnetic resonance. Another phase involves a study, by various means, of the effects of irradiation on these single crystals. Efforts are devoted to a further exploration of transitions in polymers, particularly over the temperature range from 4°K to 77°K, and polymers of varying structural features and composition will be investigated. Both dynamic mechanical and dielectric measurements are being made from 4°K and such data, together with information concerning relaxation times from nuclear magnetic resonance studies carried out above 77°K, should be helpful in extending our understanding of the mechanism of secondary relaxation processes. Measurements of thermal conductivity of polymers are being continued with emphasis on effects of radiation as well as to extension of the measurements to selected polymers of interest.

Recent Publications:

- J. A. E. Kail, J. A. Sauer, and A. E. Woodward, "Proton Magnetic Resonance of Some Synthetic Polypeptides," J. Phys. Chem. 66, (1962), p. 1292
- J. A. Suer, L. J. Merrill, and A. E. Woodward, "Dynamic Mechanical Studies of Irradiated Polypropylene," J. Polymer Sci. 58, (1962), p. 19
- K. S. Chan, G. Ranby, H. Brumberger and A Odajima, "NMR Measurements of Isotactic Poly (4-methyl-1-pentene)," J. Polymer Sci. 61, (1962), p. 529
- J. M. Crissman and R. D. McCammon, "Apparatus for Measuring the Dynamic Mechanical Properties of Polymeric Materials between 4°K and 300°K," J. Acous. Soc. 34, (1962) p. 1703

Recent Publications: (continued)

A. Jacobs and D. E. Kline, "Energy Deposition in Polymers by Reactor Radiation," J. Appl. Polymer Sci. 6, (1962) p. 605

James N. Lange, Jr., "Bending Wave Propagation in Rods and Plates," J. Acous. Soc. 35, (1963) p. 378

D. E. Kline and J. A. Sauer, "Nuclear Radiation Effects in Polytetrafluoroethylene," J. Polymer Sci. Part A 1, (1963) p. 1621

Contract: Pennsylvania State University, University Park,  
Pennsylvania

Contract Number: AT(30-1)-2541

Present Contract Term: April 1, 1964 through August 31, 1964

Cost to AEC: \$13,598

Contract Title: HIGH TEMPERATURE PROPERTIES OF TITANIUM AND ZIRCONIUM  
PHOSPHIDES AND RELATED REFRACTORY MATERIALS

Investigators: Karl A. Gingerich

Scope of Work:

The purpose of the present research is the investigation of high temperature properties of transition metal phosphides with emphasis on those of group IV.

The emphasis of research will be on the thermodynamic and structural properties of selected phosphides of the actinides, lanthanides and group IV-VI transition metal phosphides with particular attention to those of thorium, uranium, zirconium, titanium, molybdenum and tungsten. To aid the structural investigation of phosphides the structural properties of corresponding arsenides is anticipated. Rhenium will be included in an effort to determine its suitability as a container material.

Recent Publications:

K. S. Irani and K. A. Gingerich, "Structural Transformation of Zirconium Phosphide," J. Phys. Chem. Solids, 24, (1963) pp. 1153-1158.

Contract: Pennsylvania State University, University Park,  
Pennsylvania

Contract Number: AT(30-1)-2581

Present Contract Term: June 1, 1964 through May 31, 1965

Cost to AEC: \$110,893

Contract Title: FUNDAMENTAL STUDIES IN HIGH TEMPERATURE MATERIALS  
PHENOMENA

Investigators: M. E. Bell

Scope of Work:

Dielectric Studies

Development of instrumentation for the new non-contact method has been completed. Measurements on glass at very high pressure show clear electrical changes on densification. Studies of calcium yttrium fluoride crystals give the first clear evidence of dipolar relaxation, and promise a deeper insight into defect pair reorientation. Pyroelectric work has given new information on the polarization process in barium niobate zirconates.

Magnetic Measurements

A major reorganization of instrumentation has been completed, giving the laboratory excellent facilities for magnetic susceptibility and E.P.R. measurements. Preliminary results on the titanium oxides illustrate the potential of these methods.

Optical Studies

A survey of infrared spectra in simple oxides, including the influence of polymorphism, has been completed. The results show the usefulness of this technique for characterizing oxide materials.

Elastic Properties

Instrumentation for the pulse superposition method of measuring elasticity has been completed. Measurements of third order constants in silica glass and MgO crystals are in progress.

Resistivity Studies

D.C. resistivity measurements on  $ZnO-Cr_2O_3$  show a clear correlation with the extent of reaction, both resistance and reactivity are markedly influenced by the gaseous atmosphere. Combined A.C. and D.C. studies on  $Fe_2O_3$  compacts have produced a new adequate treatment of the laminar Maxwell-Wagner materials.

**Contractor:** Pennsylvania State University, University Park, Pennsylvania

**Contract Number:** AT(30-1)-2781

**Present Contract Term:** May 1, 1963 through April 30, 1964

**Cost to AEC:** \$21,053

**Contract Title:** THERMODYNAMIC PROPERTIES OF SOLID SOLUTIONS AT HIGH TEMPERATURES

**Investigators:** Arnulf Muan

**Scope of Work:**

The present research deals with experimental determination and theoretical interpretation of activity-composition curves for components in solid solutions at high temperatures. Oxide solid solutions of periclase-, spinel-, olivine- and pyroxene-types as well as binary alloy phases consisting of one noble metal (Pt or Pd) and one non-noble metal (Co or Ni) are being investigated by thermogravimetric-, quenching- and EMF-techniques.

The activity-composition curves for the solid solutions CoO-MgO, CoO-MnO, CoO-"FeO" and "FeO"-MnO with periclase-type structure and for the solid solutions  $\text{Co}_3\text{O}_4\text{-Mn}_3\text{O}_4$  and  $\text{Co}_3\text{O}_4\text{-Fe}_3\text{O}_4$  with spinel-type structure have been delineated. The stability of fayalite ( $\text{Fe}_2\text{SiO}_4$ ) and the instability of ferrosillite ( $\text{FeSiO}_3$ ) have been determined at 1000-1300°C as a basis for studies of olivine- and pyroxene-solid solutions.

It is proposed to continue the studies of olivine and pyroxene solid solutions during the coming year, as well as to complete a study of thermodynamic properties of iron-manganese spinels presently in progress. The following olivine-type solid solutions will be investigated:  $\text{Co}_2\text{SiO}_4\text{-Fe}_2\text{SiO}_4$ ,  $\text{Co}_2\text{SiO}_4\text{-Mn}_2\text{SiO}_4$ ,  $\text{Fe}_2\text{SiO}_4\text{-Mn}_2\text{SiO}_4$ . The following pyroxene-type solid solutions will be investigated:  $\text{MgSiO}_3\text{-FeSiO}_3$ ,  $\text{MnSiO}_3\text{-FeSiO}_3$ .

**Recent Publications:**

E. Aukrust and A. Muan, "Phase Relations in the System Cobalt Oxide-Manganese Oxide in Air," Journal of the American Ceramic Society, Vol 46, No.10, 1963.

E. Aukrust and A. Muan, "The Stabilities of  $\text{CoO} \cdot \text{Al}_2\text{O}_3$ ,  $\text{CoO} \cdot \text{Cr}_2\text{O}_3$ , and  $2 \text{CoO} \cdot \text{SiO}_2$ ," Vol. 46, No. 7, 1963.

Contractor: Pennsylvania State University, University Park,  
Pennsylvania

Contract Number: AT(30-1)-2887

Present Contract Term: October 1, 1963 through September 30, 1964

Cost to AEC: \$9,056

Contract Title: THE PREPARATION, PROPERTIES, AND STRUCTURE OF  
CARBONATE GLASSES

Investigators: O. F. Tuttle

#### Scope of Work:

Research on volatile-containing glasses are being carried out with three principal emphases: 1) determination of solubilities of gases in various glass compositions and defining conditions (p,t,x) of glass formation under high pressures, 2) measurement of structure-sensitive properties, and 3) determination of stability of the glasses formed.

Investigations are being continued on conditions of glass formation in carbonates and other systems where volatile compounds are clearly network formers. Solubility of molecular H<sub>2</sub>O, CO<sub>2</sub>, A, N<sub>2</sub> and probably NH<sub>3</sub> in Na<sub>2</sub>O-CaO-SiO<sub>2</sub> and other conventional glasses are being determined as a function of pressure and temperature and comparison made with ideal behavior.

Structure-sensitive measurements on the glasses formed are being continued and extended in an attempt to determine the role of the volatiles in the structure. Refractive index, infra-red absorption spectra, X-ray diffraction and low-angle scattering, as well as dielectric properties, are expected to yield information on structural groups present in the glass. Visible absorption and reflectance spectra are being obtained where suitable, and electron microscope replicas are being made to study surface properties.

Stability of glasses formed, with respect to devitrification and loss of volatiles are being determined by use of gradient heating and thermogravimetric techniques.

**Contract:** Pennsylvania, University of, Philadelphia, Pennsylvania

**Contract Number:** AT(30-1)-1893

**Present Contract Term:** February 1, 1964 through January 31, 1965

**Cost to AEC:** \$17,800

**Contract Title:** STUDY OF ALLOYS BY ELECTRON TRANSMISSION MICROSCOPY

**Investigators:** Norman Brown

**Scope of Work:**

The purpose of the research is to determine the mechanism(s) by which the martensitic transformation takes place. The primary observations will be made by electron microscopy. The effort will be centered on the very earliest stages of transformation. Evidence has been obtained that indicates that vacancies, dislocations or faults influence the  $M_s$  temperature; the influence of defects on nucleation will be examined. Most of the work will be done on an Fe-31% Ni alloy because it has a convenient  $M_s$  temperature of about  $-32^{\circ}\text{C}$ .

AuCd is also being investigated as an example of single boundary transformation. It is proposed to examine the transformation under the hot stage of the electron microscope. The martensite in AuCd is heavily twinned since the lattice invariant shear during the martensite transformation is twinning. It is planned to observe the twinning and detwinning of the twins under stress by means of the deformation stage in the electron microscope. This results will be correlated with the hysteresis loss during twinning and detwinning which is being measured by a microstrain technique.

It is also proposed to observe the martensitic transformation that is induced by a large hydrostatic tension component of stress. It is planned to produce the large hydrostatic tension by tensile shock loading. The effects of shock loading per se are being studied on another project so that the basic shock deformation can be separated from the shock induced transformation.

**Recent Publications:**

S. Dash and N. Brown, "An Investigation of the Origin and Growth of Annealing Twins," Acta. Met., Vol. 11, September 1963.

**Contractor:** Pittsburgh, University of, Pittsburgh, Pennsylvania

**Contract Number:** AT(30-1)-647

**Present Contract Term:** September 1, 1963 through August 31, 1964

**Cost to AEC:** \$46,837

**Contract Title:** ALLOY AND COMPOUND STRUCTURES AND PROPERTIES

**Investigators:** W. E. Wallace and Raymond S. Craig

**Scope of Work:**

Lanthanide hydrides having compositions represented by the formula  $AH_x$  have been prepared and studied. Here A represents Pr, Nd, Sm, Eu, Gd, Tb, Dy, Er, Tm, and Yb; and x varies from 2 to 3. Magnetic susceptibilities have been measured at various temperatures to ascertain whether or not these materials form cooperative magnetic structures. Generally the fully hydrogenated materials fail to order magnetically ( $EuH_2$  is an exception) but the incompletely hydrogenated materials order either antiferromagnetically or ferromagnetically at reduced temperatures (below 50°K). Neutron diffraction has been used to study TbD and HoD. The former orders antiferromagnetically in a sinusoidally modulated structure. The latter does not order; neutron diffraction was used here to locate the deuteride ions. Structure analysis shows that HoD<sub>3</sub> is trigonal, belonging to space group  $P\bar{3}c1$ . The constitution and magnetic characteristics of the V-H system have also been studied, the results being described in toto in the Journal of Chemical Physics, 36, 2059 (1962).

Tb-Y, Dy-Y, and Ho-Y solid solutions have been prepared by levitation melting techniques. Studies of their bulk magnetic properties indicate that diluting these lanthanides with yttrium leads to complex magnetic behavior but that generally the effect is to suppress the tendency for ferromagnetic ordering. This is also true for antiferromagnetic ordering but to a lesser extent.

Other studies include order-disorder transformations in Cd-rich Mg-Cd alloys, published in toto in Trans. AIME, 227, 26 (1963) and structural and magnetic studies of  $TiFe_2$ - $ZrFe_2$  and  $ZrCo_2$ - $ZrFe_2$  alloys, J. Chem. Phys., in press.

At present work is in progress dealing with (1) the electrical conductivity of  $EuH_2$  and (2) the magnetic properties of lanthanide nitrides. It is the intention to examine the lanthanide nitride series in a fashion similar to that

employed in recent years in the studies of the several lanthanide hydrides. Work to be undertaken includes the following topics: (1) heat capacities on  $\text{NdH}_2$  (4 to  $300^\circ\text{K}$ ) to obtain Third Law Entropy, evidence of crystal field effects, etc.; (2) studies of magnetic behavior of lanthanide-manganese Laves phases: and (3) heat capacities ( $1-4^\circ$ ) of Laves phase containing lanthanides combined with Fe, Co, and Ni to evaluate the nuclear hyperfine field.

Recent Publications:

R. L. Zanowick and W. E. Wallace, "Ferromagnetism in  $\text{EuH}_2$ ." Phys. Rev., 126, (1962) 536.

R. L. Zanowick and W. E. Wallace, "Constitution and Magnetic Susceptibilities of Vanadium-Hydrogen Alloys, " J. Chem. Phys. 36, (1962) 2059.

P. Kofstad, R. A. Butera and R. S. Craig, "Apparatus for the Continuous Recording of Internal Friction," Rev. Sci. Instruments, 33, (1962) 850.

G. S. Kamath, R. S. Craig and W. E. Wallace, "Order-Disorder Transformation in Cd-Rich Mg-Cd Alloys, " Trans. AIME, 227, (1963) 26.

S. Weinstein, R. S. Craig and W. E. Wallace, "Structural and Magnetic Characteristics of Dysprosium-Yttrium Solid Solutions," J. App. Phys. 34, (1963) 1354.

Y. Kubota and W. E. Wallace, "Magnetic Characteristics of Praseodymium, Neodymium and Samarium Hydrides," J. App. Phys. 34, (1963) 1348.

D. E. Cox, G. Shirane, W. J. Takei and W. E. Wallace, "Magnetic Structures of  $\text{TbD}_2$  and  $\text{HoD}_2$ , " J. App. Phys. 34, (1963) 1352.

W. E. Wallace, J. Kubota and R. L. Zanowick, "Magnetic Characteristics of Gadolinium, Terbium and Ytterbium Hydrides in Relation to the Electronic Nature of Lanthanide Hydrides." Advances in Chemistry Series, 39, (1963) 122

**Contract:** Pittsburgh, University of, Pittsburgh, Pennsylvania

**Contract Number:** AT(30-1)-3402

**Present Contract Term:** June 1, 1964 through May 31, 1965

**Cost to AEC:** \$87,565

**Contract Title:** MAGNETO-THERMODYNAMICS OF PARA- AND ANTIFERROMAGNETS

**Investigators:** R. A. Butera

**Scope of Work:**

The ultimate objectives of the research are essentially two-fold: first, and specifically, the direct determination of the strength of the exchange interaction in selected magnetic systems, i.e., those in which magnetic ordering occurs below 4 °K; second, and more generally, the study of the magneto-thermodynamics of selected salts containing transition metal ions and other systems as, for example, metals or intermetallics which exhibit appropriate cooperative magnetic effects at very low temperatures. These objectives, when achieved, will help provide information needed for the detailed understanding of magnetic substances at very low temperatures and under the influence of high magnetic fields, conditions which are known to exist in deep outer space.

The following measurements will be undertaken on a spherical single crystal of  $\text{MnBr}_2 \cdot 4\text{H}_2\text{O}$ :

1. Heat capacity determinations in the region 0.2-4.2°K, employing the standard procedure of introducing heat and measuring the attendant temperature rise, as a function of the applied magnetic field and the crystal orientation.
2. Magnetic moment determinations by the vertical translation of the sample along the coil axis of a superconducting solenoid as a function of the applied magnetic field and crystal orientation in the region 0.2-4.2°K
3. Magnetic entropy determinations.

**Contract:** Puerto Rico Nuclear Center, Mayaguez, Puerto Rico

**Contract Number:** AT(40-1)-1833

**Present Contract Term:** July 1, 1963 through June 30, 1964 (FY-1964)

**Cost to AEC:** \$135,000

**Contract Title:** NEUTRON DIFFRACTION STUDIES OF THE STRUCTURAL ROLE OF HYDROGEN IN CRYSTALS AND OF MAGNETIC SPIN ARRANGEMENTS IN INORGANIC CRYSTALS

**Investigators:** I. Almodovar, with guest scientists, B. Chalmers Frazer, H. J. Bielen, K. Okada, and M. I. Kay

**Scope of Work:**

The neutron diffraction group at the Puerto Rico Nuclear Center has worked on essentially two types of problems. The first is concerned with the chemical binding of atoms in crystals and molecules, mainly the role played by hydrogen and oxygen in certain important compounds. A refinement of the structure of  $\text{CaWO}_4$ , a material which shows interesting laser properties, has been completed and the results have been published. The second problem is related to the nature of ferromagnetism and antiferromagnetism in inorganic salts. Neutron diffraction measurements have been made of polycrystalline samples of  $\text{CuSO}_4$  and  $\text{Fe}_2\text{SiO}_4$ . The structure of antiferromagnetic  $\text{CuSO}_4$  has been determined, and a tentative structure for  $\text{Fe}_2\text{SiO}_4$  (fayalite) have emerged. Measurements of single crystals of  $\text{Fe}_2\text{SiO}_4$  continue to be made so as to elucidate its magnetic structure.

A structural determination of the role of hydrogen and oxygen in copper formate tetrahydrate has been initiated. Large single crystals of this compound have been grown from saturated solutions of copper carbonate in 30 % formic acid. Since copper formate also shows very interesting magnetic properties, an investigation of its magnetic structure will follow the structural investigation. Attempts will be made to establish the magnetic structure of copper chromite. Similar compounds such as  $\text{Cu FeO}_2$  have been found to yield very complicated neutron diffraction patterns.

Techniques of single crystal growth at temperatures well below room temperature are being refined in order to study the crystal structure of compounds such as methanol, dimethyl acetylene, formamide and diamonia hydrate.

Contractor: Puerto Rico Nuclear Center, Rio Piedras, Puerto Rico

Contract Number: AT(40-1)-1833

Present Contract Term: July 1, 1963 through June 30, 1964

Cost to AEC: \$28,650

Contract Title: STUDY OF RADIATION DAMAGE IN ORGANIC CRYSTALS USING ELECTRICAL CONDUCTIVITY

Investigators: Amador Cobas and H. Harry Szmant

Scope of Work:

This project is concerned with the effects of radiation on organic crystals. At present the effect of neutron irradiation on the electrical conductivity of anthracene is being studied. Similar studies will be made irradiating anthracene crystals with gamma and x-rays.

The initial stage of this investigation has been limited to the study of the changes in dark and photoconductivity in anthracene crystals produced by neutron bombardment. This type of irradiation may produce a single type of defect, namely, the knocking out of a proton from the anthracene molecule. It is likely that a result of the neutron bombardment will be the concomitant formation of a more highly condensed aromatic system and it is planned to investigate this possibility.

Electrical conductivity is very sensitive to the presence of impurities or defects and our results show that it is possible to detect quantitatively radiation damage due to neutron irradiation of anthracene crystals at levels far lower than those that can be observed by other chemical or physical techniques.

The relevant experimental results are the following: (a) neutron irradiation produces a significant increase in the conductivity of thin crystals (10-50  $\mu$ ) when measured by means of the NaI-I<sub>2</sub> electrode and a 4360A light source but not so when measured by means of the Na<sub>2</sub>SO<sub>4</sub> electrodes and a 3650A light source (b) the exalted conductivity decreases gradually to normal preirradiation levels (c) neutron irradiation does not appear to induce exalted conductivity in thick crystals (0.3 mm) even when the measurements are carried out by means of the iodine electrode. These results seem to indicate that the exalted conductivity depends on a surface phenomenon that involves an anthracene species "activated" by the neutron irradiation and an "activated" iodine species produced by the 4360A light source.

Similar studies will be made with other organic crystals.

Recent Publications:

Radiation Damage in Organic Crystals - Progress Summary Report No. 1  
(PRNC Publication No. 21)

Contract: Purdue University, Lafayette, Indiana

Contract Number: AT(11-1)-125

Present Contract Term: April 1, 1964 through March 31, 1965

Cost to AEC: \$73,399

Contract Title: BASIC RADIATION DAMAGE STUDIES

Investigators: H. M. James and J. W. MacKay

Scope of Work:

The work is a continuation of investigations which have the purpose of illuminating the basic processes of radiation damage in semiconductors, particularly germanium and silicon. To this end, most of the work involves irradiation of specimens at liquid helium temperature followed by annealing studies. The techniques used in detecting the defects and determining their properties include: D.C. conductivity and Hall measurements, calorimetric measurements of stored energy release as defects anneal, hot carrier measurements, optical excitation of electrons on defects, and electron spin resonance measurements. At present much of the work is aimed at obtaining information about a specific defect in germanium. This defect is one that is found after irradiation at liquid helium temperature and anneals at 65 K. This unstable defect appears to play a crucial role in the production of defects that are stable at higher temperatures. It apparently acts as an intermediate state in the production of more stable defects, and an understanding of its properties is vital to a correct understanding of the process of defect formation in germanium. The electronic state associated with the defect is involved in the irradiation and annealing behavior of the defect. Direct measurements of the energy of this state in the forbidden band and of its cross-section for trapping carriers are being undertaken. A study of the behavior of silicon under irradiation at liquid helium temperature has been begun.

Recent Publications:

J. W. MacKay and E. E. Klontz, "The Role of Carriers in the Displacement Process in Germanium," Radiation Damage in Solids, Vol. III, (1963) pp. 27-36.

E. E. Klontz and J. W. MacKay, "Production and Alteration of Effects Induced by Electron Irradiation of Germanium," Proceedings of the International Conference on Crystal Lattice Defects, 1962, Conference Journal of the Physical Society of Japan, Vol. 18, Supplement III, (1963), pp. 216-221.

**Contract:** Purdue University, Lafayette, Indiana

**Contract Number:** AT(11-1)-359

**Present Contract Term:** December 1, 1963 through November 30, 1964

**Cost to AEC:** \$11,556.00

**Contract Title:** DIFFUSION IN LIQUIDS AND SOLIDS

**Investigators:** Richard E. Grace

**Scope of Work:**

The current research programs can be classified into two main categories. The first deals with volume diffusion in ternary metallic solid solutions and in oxide semiconductors, and the second category deals with heterogeneous gas-solid reactions. The following problems are being studied:

1. Diffusion paths and interdiffusion coefficients are being investigated in copper-rich solid solutions of copper-zinc-manganese alloys. Experimental work on diffusion of zinc and manganese from the vapor phase into copper disks has begun.

2. Reduction of metal oxides under conditions not far removed from equilibrium will be studied with a gravimetric microbalance technique. Reduction of wüstite in damp hydrogen will be investigated under conditions where the Gibbs free energy change will be the order of 1 Kcal/mole or less.

3. Diffusion of vacancies and chemical impurities will be studied in metal oxides, such as MgO and ThO<sub>2</sub>, and the Seebeck coefficients will be measured. The motion of pores and inert markers in UO<sub>2</sub> in a temperature gradient will also be investigated. Particular attention will be paid to impurities and gas environments which control the type and concentration of defects in the oxide lattices.

**Contract:** Rensselaer Polytechnic Institute, Troy, New York

**Contract Number:** AT(30-1)-1044

**Present Contract Term:** December 1, 1963 through November 30, 1964

**Cost to AEC:** \$35,320.00

**Contract Title:** ANISOTROPIC DIFFUSION AND ELECTROMIGRATION

**Investigators:** H. B. Huntington

**Scope of Work:**

This work on atom movements follows two main channels. One of these deals with classical diffusion studies in non-cubic metals. Recently we have been investigating the diffusion of impurities in zinc and have found that those elements with  $Z < 2$  diffuse more slowly than zinc itself, while those elements whose  $Z$  is greater than 2 diffuse more rapidly and with an anisotropy of reverse sign. That is, they diffuse more rapidly in the basal plane than along the C-axis. Qualitatively this observation can be understood in terms of the vacancy mechanism. From the fact that the diffusion of cadmium in zinc is also faster than self-diffusion, we have inferred that the diffusion of zinc in cadmium should be slower than the self-diffusion of cadmium. We have just started to explore impurity diffusion in cadmium and the first result with zinc shows that our surmise was correct. Projected work along this line includes additional impurity diffusions in both zinc and cadmium and a study of the influence of impurities on self-diffusion in both metals.

The other main line of investigation under this contract is concerned with electromigration, or the mass transport under high electric currents. We are presently investigating electromigration in silver, cobalt, and refractory metals such as zirconium. The work with cobalt has turned out to be particularly interesting since a marked Soret effect has been observed and the DC motion appears to be toward the cathode, the direction one would expect from positive charge carriers. In addition to these projects we also are interested in repeating studies of copper and in exploring electromigration in gold foil.

Recent Publications:

H. B. Huntington and Siu-Chung Ho, "Electromigration in Metals", J. Phys Soc. of Japan, 18 (1963) 202.

P. B. Ghate, "Anisotropic Diffusion of Cadmium and Gold Tracers in Zinc Single Crystals", Phys. Rev., 131 (1963) 174.

**Contract:** Rensselaer Polytechnic Institute, Troy, New York

**Contract Number:** AT(30-1)-1995

**Present Contract Term:** February 1, 1964 through January 31, 1965

**Cost to AEC:** \$30,690

**Contract Title:** THEORETICAL RESEARCH RELATING TO RADIATION DAMAGE  
IN SOLIDS

**Investigators:** Edmond Brown

**Scope of Work:**

The research deals with the behavior of electrons in crystalline potentials. One problem is concerned with the effect of uniform magnetic and electric fields. The approach makes use of the methods of group theory, taking advantage of the periodicity which exists under these conditions. A second problem is the electronic contribution to the energy of sodium when the lattice is distorted by a phonon. The results of this calculation will then be used to determine the phonon spectrum, without using any parameters. A third problem deals with the determination of the band structure of the ordered phase of the alloy  $\text{Cu}_3\text{Au}$ . In addition to these, investigations into the applicability of pseudopotential methods for the determination of band structures will be pursued as a fourth problem.

Contractor: Rensselaer Polytechnic Institute, Troy, New York

Contract Number: AT(30-1)-2159

Present Contract Term: August 1, 1963 through July 31, 1964

Cost to AEC: \$33,150

Contract Title: METALLURGICAL STUDIES OF Zr and Th AND OF THE ALLOYING BEHAVIOR OF RARE EARTH-TRANSITION METAL SYSTEMS

Investigators: W. R. Clough

Scope of Work:

The effects of rare-earth solutes including neodymium, gadolinium, holmium, erbium, and lutetium on the allotropic transformation temperatures of thorium solvent have been experimentally determined and correlated with alloy theory. The transformation temperature of thorium is raised by each of the rare earth additions, but a maximum is reached after which there is a lowering by further alloy additions until the eutectoid temperature is reached. Yttrium, neodymium, dysprosium, holmium, erbium, gadolinium, terbium, thulium, and lutetium (with the exception of neodymium) raised the allotropic transformation temperature of zirconium, thus indicating peritectoid reactions in these systems.

The individual effects of six rare earth additions on the surface tension of liquid thorium have been studied in some detail by use of the drop weight technique. The value of the surface tension of pure thorium at the melting point was determined to be  $978 \pm 32$  dynes per centimeter, and all rare-earth additions resulted in altered values. Metallographic techniques were used to determine the solid solubility of lutetium in thorium solvent, and the solubilities and the partial molar heats of mixing of Nd, Gd, Tb, Dy, Ho, Er, Lu, and Y in alpha zirconium have been calculated by model analysis, and have been compared with results obtained by calorimetry and other experimental techniques. In the future, physical metallurgy research concerned with the extent of primary solid solubility of rare earth solutes in thorium solvent will be continued, as will rare earth-rare earth studies. The effect of rare-earth solutes on the c/a ration of hexagonal zirconium solvent, and on mechanical and oxidation characteristics will be evaluated in detail.

Recent Publications:

L. Ianniello, and A. A. Burr, "Effect of Some Rare Earth Elements of the HCP-BCC Transformation of Zirconium," Jnl. of Applied Physics, Vol. 33, No. 9 (1962) pp. 2689-2690.

Recent Publications (Continued)

F. Shunk and A. A. Burr, "Surface Tension Studies of Liquid Zirconium-Rare Earth Alloys," ASM Trans., Vol. 55, (1962) p 786.

James C. Uy, and A. A. Burr, "The Solute Metallic Valence as an Index of Phase Stabilization in Zirconium-Base Alloys," Trans. A.I.M.E., Vol. 224, (1962) p. 204.

**Contract:** Rensselaer Polytechnic Institute, Troy, New York

**Contract Number:** AT(30-1)-2408

**Present Contract Term:** June 1, 1964 through May 31, 1965

**Cost to AEC:** \$21,000

**Contract Title:** STUDIES OF SINTERING

**Investigators:** Fritz V. Lenel

**Scope of Work:**

By determining the isothermal shrinkage rates of copper powder compacts in the range of 700°- 1060°C, it has been shown that under the conditions of the experiments the material transport mechanism is by dislocation climb rather than by Herring - Nabarro creep. By making model experiments in which the increase in neck area between a silver plate and a silver sphere is determined as a function of applied stress using electrical resistance as the measuring method, a quantitative insight of the range of temperatures and stresses, where this mechanism is applicable, is to be obtained.

Work on the mechanism of material transport is to be extended in two directions:

- (1) Measurements of the rate of coalescence of extremely small gold particles with a size in the range of 200 to 1000 Angstroms are to be made in an electron microscope at a range of temperatures.
- (2) The mechanism is to be studied for materials other than metals, such as ionic crystals and compounds having covalent bonds.

**Recent Publications:**

F. V. Lenel, H. H. Hausner, O. V. Roman and G. S. Ansell, "The Influence of Gravity upon the Shrinkage of Copper Powder Compacts," Trans. AIME, June, (1963).

Contract: Rensselaer Polytechnic Institute, Troy, New York

Contract Number: AT(30-1)-2714

Present Contract Term: February 1, 1964 through July 15, 1964

Cost to AEC: No-Fund Extension

Contract Title: THE ELECTROCHEMICAL AND CORROSION CHARACTERISTICS OF RARE EARTH AND YTTRIUM METALS

Investigators: Norbert D. Greene

Scope of Work:

Electrochemical and corrosion behavior of the rare earths, thorium and uranium including:

1. Oxidation behavior of the rare earths in dry and moist air and oxygen at near ambient temperatures (to 200°C) using continuous weight gain measurements.
2. X-ray and electron diffraction studies of oxide films on the rare earth metals.
3. Hydrogen overvoltage studies on rare earth metals in buffered phosphoric acid solutions.
4. Dissolution measurements of uranium, thorium, and their alloys using potentiostatic techniques.

**Contractor:** Rensselaer Polytechnic Institute, Troy, New York

**Contract Number:** AT(30-1)-3004

**Present Contract Term:** April 1, 1964 through March 31, 1965

**Cost to AEC:** \$21,993

**Contract Title:** DENDRITE GROWTH IN SUPERCOOLED METALS

**Investigators:** Wylie J. Childs

**Scope of Work:**

Measurements of dendritic growth velocities of supercooled metals and alloys will be done. These metals include the lower melting point metals that are easily super-cooled, such as bismuth and tin and their alloys. The effect of solute build-up in front of the advancing interface for alloys with different amounts of solid solubility will be studied to see the influence on dendrite growth rate.

Fine wire thermocouples will be used with high response galvanometers to measure the thermal gradient in front of the advancing dendrite in an attempt to obtain a more accurate value for the temperature at the tip of the growing dendrite.

The influence of the surface upon which growth occurs, such as a Pyrex crucible wall, will be studied for its effect on velocity. With rhombohedral bismuth, the velocity of dendrite growth is much greater when in contact with a Pyrex surface.

Currently employed techniques will be modified in an effort to study the effect of supercooling and alloying on the morphology of dendrites for the higher melting point metals such as nickel and iron.

Contractor: Rensselaer Polytechnic Institute, Troy, New York

Contract Number: AT(30-1)-3030

Present Contract Term: August 1, 1963 through July 31, 1964

Cost to AEC: \$21,180

Contract Title: NUCLEAR QUADRUPOLE COUPLING STUDIES IN SOLIDS

Investigators: Philip A. Casabella

Scope of Work:

Nuclear quadrupole coupling studies are being conducted in four areas:

1) The Group III Halides. These compounds will be studied in an effort to gain information about their molecular and crystalline structure.

2) Ferroelectrics. The quadrupole coupling of  $\text{Na}^{23}$  in Rochelle Salt will be completed in order to learn what types of chemical bonds exist in the material, and what role they play in ferroelectric phenomena.

3) Effects of  $\text{Co}^{60}$  Radiation. By studying the effects of  $\text{Co}^{60}$  gamma rays on nuclear quadrupole coupling it will be possible to get detailed information about the damage that the gamma rays are doing to the crystal structure.

4) Nuclear Quadrupole Coupling of Nitrogen. There still remain some details of the theory of nuclear quadrupole coupling of nitrogen which have not been worked out for the case of large asymmetry of the coupling. This area will be investigated both theoretically and experimentally.

**Contract:** Rensselaer Polytechnic Institute, Troy, New York

**Contract Number:** AT(30-1)-3176

**Present Contract Term:** March 1, 1964 through February 28, 1965

**Cost to AEC:** \$20,211.00

**Contract Title:** PRECIPITATION PHENOMENA IN CERAMICS: THE  
SYSTEM  $\text{BaTiO}_3\text{-CaTiO}_3$

**Investigators:** Robert C. DeVries and George S. Ansell

**Scope of Work:**

Homogeneous solid solutions in the system  $\text{BaTiO}_3\text{-CaTiO}_3$  will be prepared and then heat-treated in the two-phase precipitation region. The kinetics and crystallography of the precipitate structures will be described and interpreted, using metallographic techniques. The correlation of the precipitate structure with such dielectric properties as capacitance and capacitance change with time will be attempted.

Contract: Rensselaer Polytechnic Institute, Troy, New York

Contract Number: AT(30-1)-3340

Present Contract Term: March 1, 1964 through February 28, 1965

Cost to AEC: \$17,680

Contract Title: DIFFUSION AND ELECTRICAL CONDUCTIVITY IN CRYSTALLINE AND GLASSY CALCIUM SILICATES

Investigators: John D. Mackenzie

Scope of Work:

The objectives of this research are: (a) to investigate the electrical conductivity of  $\text{CaO.SiO}_2$  glasses as functions of calcium concentration and of sodium impurities; (b) to prepare single crystals of calcium metasilicate and to measure its electrical conductivity; and (c) to measure the diffusion coefficient of Ca ion in the glasses and in the crystals. One important reason for this work is because the specific volumes of the crystal and the glass of similar composition are equal. Correlation of ionic motions in a disordered and an ordered solid of identical specific volumes and chemical composition is necessary in the understanding of many physical properties of glasses.

Glasses will be prepared by the fusion of calcium carbonate and pure silica sand. Crystals will be prepared by direct seeding of the melt or growth from flux. For the diffusion work,  $\text{Ca}^{45}$ , a weak beta-emitter having a half-life of one hundred and sixty-five days will be used. The d.c. electrical conductivity will be measured by conventional electrometers suitable for high resistivity samples. The amounts of sodium impurities will be adjusted by the controlled addition of sodium carbonate before melting.

**Contract:** Rochester, University of, Rochester, New York

**Contract Number:** AT(30-1)-3388

**Present Contract Term:** May 15, 1964 through May 14, 1965

**Cost to AEC:** \$35,000

**Contract Title:** RESEARCH IN MAGNETIC RESONANCE

**Investigators:** T. G. Castner

**Scope of Work:**

The exponential temperature-dependent relaxation of shallow donors is thought to depend on the impurity spin-orbit interaction (particularly for the heavier donors). For the exponential range there are several types of relaxation mechanisms, all involving the spin-orbit interaction. Combined static strain and spin-lattice relaxation rate experiments may allow the determination of the correct mechanism. Static strains could readily produce drastic effects on the spin-lattice relaxation rate when the energy splitting of the conduction band valleys due to the strain is comparable to or larger than the spin-orbit splitting. It is also planned to investigate the magnetic field dependence of the relaxation rates in the exponential temperature-dependent region. Another line of investigation would be the study of relaxation processes for deeper donors,  $S^+$  being an attractive example.<sup>(9)</sup> In addition, there are several 3d ions of various charge states in substitutional sites in Si. Some of these may well have exponential temperature-dependent relaxation.

The self-trapped hole (halogen molecule ion, e.g.,  $Cl_2^-$ ), the H center, (an interstitial Cl atom), and the substitutional oxygen molecule ion  $O_2^-$  in the alkali halides all have extra degrees of freedom associated with them. Because of the anisotropic g-factors and hyperfine interaction constants, it is possible that the extra rotational degrees of freedom of these molecule ions locked in the lattice and their interaction with the lattice waves may be dominant mechanisms for the spin-lattice relaxation of these paramagnetic defects. Almost all the spin-lattice relaxation effort has been on paramagnetic defects with point symmetry. It is therefore of some interest to study the spin-phonon interactions of these paramagnetic diatomic molecule ions in various alkali halides.

Feher and Clark have demonstrated the possibility of polarizing  $Sb^{123}$ ,  $Sb^{121}$ , and In nuclei with a dc current by heating the conduction electrons above the lattice temperature. It is planned to study nuclear polarization and also nuclear spin-lattice relaxation effects in the presence of hot carriers for nuclei with spin  $I = \frac{1}{2}$  to avoid competing quadrupolar relaxation effects and also to attempt these experiments in samples free of paramagnetic impurities with strong spin-lattice relaxation rates.

Contractor: RIAS, Baltimore, Maryland  
Contract Number: AT(30-1)-2531  
Present Contract Term: August 1, 1963 through July 31, 1964  
Cost to AEC: \$30,100  
Contract Title: INVESTIGATIONS OF ALLOTROPIC TRANSFORMATION IN METALS

Investigators: H. M. Otte

Scope of Work:

Work presently under way includes: (1) Determination of the Burgers vectors of dislocations in the martensite. (2) Determination of the Burgers vectors of dislocations in the austenite-martensite interface. (3) Observation of the formation of martensite and epsilon on cooling in the electron microscope. (4) Factors affecting the nucleation and transformation of crystal structures in general. (5) The effect of radiation damage on allotropic transformations. (6) Correlation between physical and mechanical effects of allotropic transformations and the structural features observable by electron microscopy. (7) A study of the correspondence in the  $\gamma \rightarrow \alpha$  and  $\beta \rightarrow \alpha$  transformation in Uranium and its alloys. A more detailed investigation than carried out by Lomer. (8) Theoretical investigation of possible dislocation interactions that may play a role in the low temperature transformation of mercury.

Recent Publications:

J. Dash and H. M. Otte, "Thin Film Transmission Observations of Athermal Transformation in Stainless Steel," Fifth International Congress for Electron Microscopy, Philadelphia, 1962, vol. 1, paper HH-4, Academic Press, N. Y., and London.

H. M. Otte, "Determination of the Dilation Parameters in Martensitic Transformations," Acta Cryst., 1963, 16, 8.

J. Dash and H. M. Otte, "The Martensite Transformation in Stainless Steel," Acta Met., in press.

M. P. Drazin and H. M. Otte, "The Systematic Determination of Crystallographic Orientations from Three Octahedral Traces on a Plane Surface" Phys. Stat., Sol., 1963, 3 (#6)

**Contract:** Rutgers, The State University, New Brunswick,  
New Jersey

**Contract Number:** AT(30-1)-3384

**Present Contract Term:** June 1, 1964 through May 31, 1965

**Cost to AEC:** \$28,545

**Contract Title:** RELAXATION BEHAVIOR, MOLECULAR MOTION AND STRUCTURE  
IN POLYMERS AND RELATED MATERIALS

**Investigators:** J. A. Sauer

**Scope of Work:**

In this proposed study of relaxation behavior and molecular motion in polymers and related materials, existing and new data concerning internal transitions in polymers will be studied and analyzed in an attempt to relate experimentally observed low temperature transitions more directly to specific features of polymer structure. Consideration will be given to structural information and to known or estimated values of energy barriers to segmental rotation as well as to mechanical relaxation data, nuclear magnetic resonance data and dielectric data, where available. The proposed experimental studies will involve construction of a sensitive measuring apparatus for investigation of relaxation behavior over a wide temperature range. Some of the problems to be studied are the effect of radiation on polymers having side chain crystallinity, the effect of low molecular weight ingredients, such as monomer and water, and the effect of specific chain substitutions on the relaxation spectrum. Another aspect of the experimental studies will involve growth of crystals of various poly-alpha-olefins from dilute solutions of purified, isotactic polymer and study of the resulting crystal structures by means of X-ray and electron diffraction techniques.

Paul W. McDaniel, Director  
Division of Research

August 25, 1964

M. C. Wittels  
Metallurgy and Materials Programs

NEW CONTRACT WITH ST. MARY'S COLLEGE--(MORGAN/BLASS).

This research proposal is entitled "Experimental Study of the Structure and Electronic Properties of Single Crystal Molybdenum and Tungsten Ribbons". It is most directly concerned with single crystal refractory metal surfaces and the relation between thermally-induced surface disorder and thermionic emission.

Several experimental techniques will be utilized including optical microscopy, electron microscopy, low energy electron diffraction (LEED), single crystal growth and preparation, x-ray diffraction, and retarding potential measurements.

The single crystal refractory crystals will be obtained in two ways: (a) grown by the strain-anneal method, and (b) commercially available ingots. In either case desired orientations will have to be cut and surfaces prepared, and although the initial studies will be on clean metal surfaces, thermionic emission and LEED studies are planned for adsorbed films.

Quantitative studies of surface thermal disorder have not been fully established with the LEED technique and in this program a concerted effort will be made to achieve these ends.

Thermionic emission constants will be measured by the retarding potential technique using plane parallel geometry and a magnetic field to collimate the electron beam. In these same experiments the reflection coefficients, empirical work functions, and Richardson  $A$  values can be measured. By the combination of the emission measurements and a clearer understanding of real surface structures it is expected that a definitive correlation will result.

The reflection coefficients will be measured for low accelerating fields, one volt or less, and these data will be compared with results calculated for recently proposed potential models of a metal surface.

Recent results of Zolweg (J. Appl. Phys. 34, 2590 (1963)) indicate that early measurements of reflection coefficients could be in error by a factor of two or five. In order to clarify this point an investigation will be made on the effect of multiple reflections on the reflection coefficients.

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August 25, 1964

To accomplish this a retarding potential tube similar to the one designed by Ebelton (Phys. Rev. 107, 1553 (1957)) is being constructed and is well under way. The LEED tube is also near completion and is presently being tested.

Professor Morgan has wisely accepted the free offer of services and consultation from faculty experts at the Universities of Minnesota and Notre Dame to complement the capability at St. Mary's. The free use of electron microscope and computer facilities at IBM (Rochester, Minn.) are also available.

This proposal has been favorably reviewed with ratings from fair to excellent by Farnsworth (Brown), Gomer (Chicago), Lender (Bell Labs), Danforth (Franklin Inst.), Germer (Cornell), Huntington (RPI), Young (NBS), and Coomes (Notre Dame).

The research is definitely in AEC interests and support is recommended as indicated in the budget.

AEC funds	\$25,000	
St. Mary's funds	11,755	(32%)
Total	\$36,755	

Title to the equipment should be vested in the college since its contribution exceeds its value.

Professors Morgan and Blass have no federally supported research contracts.

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**Contract:** Southern California, University of, University Park,  
Los Angeles 7, California

**Contract Number:** AT(11-1)-113

**Present Contract Term:** January 1, 1964 through December 31, 1964

**Cost to AEC:** \$53,385

**Contract Title:** A STUDY OF MAGNETIZATION, THERMAL, AND TRANSPORT CURRENT  
PHENOMENA IN HIGH FIELD SUPERCONDUCTORS

**Investigators:** Marcel LeBlanc

**Scope of Work:**

The magnetic, critical current, and resistive behavior in high field superconductors will be correlated utilizing transport current as a controlled variable. Here the state of magnetization is observed by ballistically measuring the emf induced in pick up coils surrounding the superconductor as it is raised above its transition temperature by a heat pulse. The magnetic and transport current phenomena will be studied as a function of temperature in high field superconductors.

A search will be made for bulk properties by measuring the slope and change of slope of initial diamagnetic magnetization factor in a longitudinal field as the specimen cross-section is lowered.

Artificial filamentary superconductors (soft) will be prepared and their critical current behavior measured as a function of magnetic field intensity and orientation.

Increases will be examined in current carrying capacities of hard superconductors over given ranges of external field. In particular this will be examined by the method of electron tunnelling in thin films as a function of transport current.

Nuclear orientation effects will be utilized to examine the energy vortex model. Here it is proposed to introduce paramagnetic impurities in situ, by neutron capture, and to monitor the average magnetization of these impurities through the anisotropic emission of gamma radiation. The effects of attendant radiation damage will also be explored.

The influence of transport current and macroscopic diamagnetic and paramagnetic induced currents on the thermal conductivity and specific heat of ideal and non-ideal type II superconductors, (Nb, NbTa, NbZr) will be studied. These effects will be followed in wires as a function of temperature and applied longitudinal and transverse fields.

**Contractor:** Stanford University, Stanford, California

**Contract Number:** AT(04-3)-283

**Present Contract Term:** August 1, 1963 through July 31, 1964

**Cost to AEC:** \$26,400

**Contract Title:** THERMODYNAMIC AND TRANSPORT PROPERTIES IN LIQUID METAL SOLUTIONS

**Investigators:** David A. Stevenson

**Scope of Work:**

Thermodynamic Properties of Liquid Metal Solutions: The thermodynamic activities and excess enthalpies of solution are being experimentally determined for the components of selected binary liquid metal alloys. For systems in which the solid phase dissolves only to a limited extent in the liquid phase, the solid-liquid phase distribution of the components is determined. For systems exhibiting a broad solubility range, the vapor pressure of one of the components over the liquid alloy is being measured using a Knudsen cell technique or a modified vapor density technique. This experimental information is fundamental to the understanding of the behavior of liquid metal solutions.

Thermodynamic Properties and Defect Structure of Intermetallic Compounds: The free energy of formation and the enthalpy of formation of binary intermetallic compounds is being determined by measuring the vapor pressure of the components above the compound at different temperatures. The Knudsen cell technique or a modified vapor density technique is being used for these measurements.

The stable range of composition and the influence of non-stoichiometry on the defect structure of intermetallic compounds is being investigated. The II - VI compounds are currently under investigation. In order fully to characterize the defect structure, experimental determinations of the electrical properties, the atomic mobility and the X-ray and picnometric densities are being made for compounds of different preparative history.

Contract: Stanford University, Stanford, California

Contract Number: AT(04-3)-298

Present Contract Term: August 1, 1963 through July 31, 1964

Cost to AEC: \$54,307

Contract Title: KINETICS IN SOLID STATE SYSTEMS

Investigators: Victor F. Macres and Robert A. Huggins

#### Scope of Work:

This program is directed toward achieving a more basic understanding of the mechanisms involved in diffusion-controlled solid state reactions; in particular, those involving mass transfer at high solute concentrations and over large compositional regions. Included in this study are the dependence of diffusion behavior on thermodynamic properties, imperfection concentration, and the presence of electrical and strain fields. Materials being studied include covalent and ionic ordered structures as well as metallic solid solutions. The program is largely experimental, some of the major techniques utilized being nuclear magnetic resonance, electron microprobe analysis, and radioactive traces analysis. Some of the current research activities are given below.

Thermodynamic properties of the systems Cu-Zn, Cu-Cd, and Cu-Cd-Zn are under study. Experiments involving vapor-solid reactions are being used to determine the composition and temperature dependence of zinc and cadmium activities. Thermodynamic quantities obtained from these data are being used to interpret diffusion behavior in alpha-Cu-Cd-Zn and  $\text{Cu}_2\text{Cd}_3$  and  $\text{Cu}_5\text{Zn}_8$ . The diffusion of various cations, including Ti, Mn, Mo, and Cr, in  $\text{Al}_2\text{O}_3$  is being investigated. Included in this study are the influence of stoichiometry  $\text{Al}_2\text{O}_3$  are being used. The formation of the spinel  $\text{MgAl}_2\text{O}_4$  from MgO and  $\text{Al}_2\text{O}_3$  and the influence of electric fields is also being studied. Finally, some attention is being given to theoretical considerations of multi-ionized impurity diffusion in semiconductor materials.

#### Recent Publications:

R. R. Dils, L. Zeitz, and R. A. Huggins, "A Suggested Secondary Fluorescence Correction Technique for Electron Probe Analyses in the Vicinity of a Steep Concentration Gradient," X-Ray Optics and X-Ray Microanalysis, Academic Press (1963).

D. R. Stiefbold, J. R. Boston, and R. A. Huggins, "A New Dislocation Etchant for Magnesium Oxide," Jour. Amer. Ceram. Soc. 46, (1963) p. 507.

Contractor: Stanford University, Stanford, California

Contract Number: AT(04-3)-326

Present Contract Term: October 1, 1963 through September 30, 1964

Cost to AEC: \$20,000

Contract Title: EFFECT OF POINT DEFECTS ON MECHANICAL BEHAVIOR OF CRYSTALLING SOLIDS

Investigators: Oleg D. Sherby

**Scope of Work:**

Evaluation of the anomalous weakness of iron during phase transformation is continuing. The results are described in a technical report, "Strength of Iron during Allotropic Transformation" (Frank Clinard and Oleg Sherby). It is suggested that the origin of transformation softening is associated with the generation of excess lattice vacancies during heating, since the nucleating gamma phase is more dense than the alpha matrix, and the generation of excess interstitial atoms during cooling, when the opposite is true. These excess point defects will contribute to creep since dislocation climb is enhanced. A new apparatus for multiple thermal cycling of Armco iron has been constructed, and transmission electron microscopy of the defect structure of iron after transformation is in progress.

Metals deformed in the  $0.6 - 0.8 T_m$  temperature range often exhibit strain softening, which refers to the tendency of metals to become weaker with increasing plastic deformation. Strain softening is believed to be associated with the creation of excess lattice vacancies during deformation. Tests under constant torsional stress have been made on Fe-25% Cr (BCC) and  $\gamma$ -phase Armco iron (FCC). The results suggest that the number of excess vacancies created is a power function of the amount of plastic deformation. By relating the diffusivity during deformation to the strain rate, it is shown that enhancements in diffusivity of up to a factor of approximately 6 result.

**Contractor:** Syracuse University, Syracuse, New York

**Contract Number:** AT(30-1)-2731

**Present Contract Term:** August 1, 1963 through July 31, 1964

**Cost to AEC:** \$43,103

**Contract Title:** PHYSICAL PROPERTIES AND ALLOYING BEHAVIOR OF ALKALI AND ALKALINE EARTH METALS

**Investigators:** F. A. Kanda and D. V. Keller, Jr.

**Scope of Work:**

In order to complete the equilibrium studies of the alkali-alkaline earth systems, the exact nature or boundaries of some restricted solid state regions of these systems remain to be settled. These are the solid solution region of the intermediate phase BaNa, and the phase transformation and solid solubility of Sr and Ca rich alloys in the Sr-Na and Ca-Li systems. Intermediate phase studies, usually by single crystal x-ray crystallographic techniques, have indicated characteristic packing clusters in these systems which are unique and require the variability in stoichiometry observed, e.g.  $\text{CaLi}_2$ ,  $\text{Sr}_3\text{Li}_2$ ,  $\text{SrMg}_4$ ,  $\text{Sr}_6(\text{MgLi})_{23}$ ,  $\text{Sr}_2(\text{MgBa})_{17}$ , etc. Studies will be initiated for the Ba-Al and possibly the Sr-Al systems to observe any correlation between the nature of these with previously investigated systems and intermediate phases, in order to note both the size and valency effect of Al in these systems. Liquid-density investigations will continue for the Mg-Sn system for all compositions above the liquidus. Density isotherms across the system as well as density-temperature curves for each composition will be studied for effects related to pre-eutectic and pre-compound solidifications. Correlations will be considered in conjunction with calorimetric studies made simultaneously for the same compositions over the same temperature ranges. Time and personnel allowing, calorimetric studies may be extended to cover transitions or reactions observed in the phase systems previously studied, e.g. the retrograde melting region of Sr rich alloys in the Sr-Li system.

**Recent Publications:**

F. E. Wang, F. A. Kanda, and A. J. King, "The Li-Sr Equilibrium System," Jnl. of Phys. Chem., 66, (1962) p. 2138.

F. E. Wang, A. J. King, and F. A. Kanda, "The Crystal Structure of  $\text{Sr}_6\text{Li}_{23}$  and  $\text{Sr}_3\text{Li}_2$ ," Jnl. of Phys. Chem., 66, (1962) p. 2142.

**Contract:** Temple University, Philadelphia, Pennsylvania

**Contract Number:** AT(30-1)-2775

**Present Contract Term:** May 15, 1964 through May 14, 1965

**Cost to AEC:** \$31,418

**Contract Title:** A SOLID STATE STUDY OF ZIRCONIUM AND NIOBIUM OXIDES

**Investigators:** Robert E. Salomon

**Scope of Work:**

Photovoltaic measurements with anodized zirconium and niobium electrodes will be continued. An attempt will be made to determine the mechanism of the anomalous high voltage photovoltaic effect at low temperatures. To accomplish this objective the photovoltage will be studied as a function of oxygen adsorption. Recent measurements have shown the importance of the ambient on the open circuit photovoltage. These measurements will be extended to liquid helium temperatures. The measurements of the short circuit photocurrents in niobium electrodes will be completed.

The reflectance spectra measurements of impurity doped zirconium oxide will be continued. Electron spin resonance measurements will be made on all samples. An attempt will be made to dope the oxide with small amounts of rare earth ions. The luminescence of the resulting materials will be measured and the crystal field perturbation of the expected line emission will be determined. These measurements and the reflectance spectra studies are designed to probe the crystal field within the oxide. Similar studies with niobium oxide have been started and will be continued.

**Recent Publications:**

P.N. Ramachandran and R.E. Salomon, J. Physics and Chemistry of Solids 24, 583-584 (1963)

R.E. Salomon, G.B. Adams and W.M. Graven, J. Electrochem. Soc. 110, 1163-1165 (1963)

**Contractor:** Temple University, Philadelphia, Pennsylvania

**Contract Number:** AT(30-1)-2812

**Present Contract Term:** August 1, 1963 through July 31, 1964

**Cost to AEC:** \$70,329

**Contract Title:** STUDY OF THE IB-IIB BETA PHASE ALLOYS

**Investigators:** Leonard Muldawer and H. Amar

**Scope of Work:**

The general purpose of this study is the advancement of our understanding of alloys, in particular the beta-brass type alloys.

1. Diffraction Studies of Structures and Transformations. The ternary alloys  $\text{AgAuCd}_2$ ,  $\text{AgAuZn}_2$  and  $\text{CuAuZn}_2$  have been shown to have the ordered Heusler alloy structure at room temperature. High temperature x-ray diffraction studies are being used to follow the noble metal disordering as the temperature is raised. The existence region for the zeta phase in gold modified AgCd is being mapped. Effects of temperature and composition on lattice constant are being obtained. Other contemplated studies include the structures in the CuZn-AuZn and AgZn-AuZn systems and electron diffraction studies of surface transformation.

2. Spectral Reflectivity and Optical Constants Measurement. Reflectivity data over an extended range (500 A to 10,000A) and optical constants over a limited range will be obtained. An ellipsometer will be used for the latter data. These data will be combined with the aid of Kramers-Kronig relations to give optical constant data over the extended range. Measurements will be taken as a function of temperature and composition. Semi-empirical theory will be utilized to interpret the results in terms of free-electron and interband effects. Early data on beta-brass of varying composition have been interpreted to give the nature of the interband transition. A variation in the interband "gap" can be used to explain the early data from CuZn, AgZn, and AuZn in a consistent fashion.

It has been established that interband transitions play a vital role in the interaction of light with metals like Ag, Cu and their alloys. A meaningful assessment of interband effects can only be based on a knowledge of the electronic structure of our alloys. Besides its intrinsic interest, and its relevance to the optical properties, this knowledge would allow a better understanding of a host of other properties such as the Hall effect, the electric and thermal conductivities, the

electronic specific heat, etc. A calculation of the band structure of beta-brass type alloys has been undertaken, based on the Green function method. This method uses the best features of the cellular method, which it combines with scattering techniques. The major computational effort is the calculation of the "structure constants." This is a distinct advantage, since the same structure constants can be used to calculate the energy bands in other alloys having the same crystal structure as beta brass. An attempt will be made to construct a plausible Fermi surface, and some of the crystal wave functions at high symmetry points of the Brillouin zones.

Recent Publications:

F. Rothwarf and L. Muldower, "Electrical Resistivity and X-Ray Diffraction Study of the Beta AgCd-AuCd System," J. of Applied Physics, 33, (1962) p. 2531.

L. Muldower, "Spectral Reflectivity as a Function of Temperature of beta-Brass Type Alloys," The Physical Review, 127, (1962) p. 1551.

**Contractor:** Tennessee, University of, Knoxville, Tennessee

**Contract Number:** AT(40-1)-1068

**Present Contract Term:** September 1, 1963 through August 31, 1964

**Cost to AEC:** \$9,936

**Contract Title:** CALORIMETRIC MEASUREMENTS ON METAL SYSTEMS

**Investigators:** E. E. Stansbury

**Scope of Work:**

The broad scope of this research is the application of dynamic adiabatic calorimetry to the measurement of thermodynamic properties of metal systems in the temperature range from room temperature to 1000°C. Related phenomena such as meta-stable states and non-equilibrium imperfection concentrations as revealed by energy absorption-temperature data are also being investigated. The experimental method yields specific heat data with an accuracy of better than + 1% up to 700°C.

One phase of the current research is concerned with measurement of the specific heat of Ni-rich alloys of the Ni-Cr and Ni-Mo alloy systems. Both of these systems show anomalies in the specific heat of the terminal solid solution which is associated with short-range order. At higher compositions in the Ni-Mo system, the Ni<sub>4</sub>Mo phase forms by a long-range ordering transformation from the terminal phase. For higher compositions in the Ni-Cr system, resistivity data suggest long-range order near 33 at % Cr. The current research will be a comparative investigation of these two systems in terms of short- and long-range order for initial states of the alloys of as-quenched and slowly cooled.

A second phase of the research will be a continuation of a study of anomalies in the specific heat of Cu-base alloys. Measurements have been completed on Cu-Al and Cu-Ga solid solutions and will be continued on systems containing Ge and As.

**Contract:** Toledo, University of, Toledo, Ohio

**Contract Number:** AT(11-1)-1000

**Present Contract Term:** February 1, 1963 through January 31, 1964

**Cost to AEC:** No-fund Extension

**Contract Title:** OXIDATION OF ZIRCONIUM-NIOBIUM ALLOYS IN THE TEMPERATURE RANGE 300-500°C

**Investigators:** Otto Zmeskal

**Scope of Work:**

The purpose of this project is to investigate the mechanism of the oxidation of zirconium-niobium alloys in the low temperature range.

An investigation will be made into the effect of total pressure on the oxidation process. Regular, smooth oxidation curves at low temperatures have been obtained by others only under conditions of low total pressure. The results of the present investigation show great irregularity at 400°C, a phenomenon displayed in many repeat runs, and have convinced us that this is a matter worth investigating.

The metallographic examinations will be continued and elaborated upon to follow the visual structural changes during the oxidation process. The change in character of the interface from a straight one to a very irregular one is an interesting phenomenon. Surface studies will throw light on the cracking that develops in the film.

Study will also be made of the development of thin oxide films on Zr and Zr-Nb alloys at low temperatures (i.e. 500°C or lower) by means of an electron microscope. It is hoped that the results from the electron micrographic examination of the films will contribute to the explanation of the irregular behavior at low temperatures.

**Contract:** Tufts University, Medford, Massachusetts

**Contract Number:** AT(30-1)-2968

**Present Contract Term:** May 1, 1964 through April 30, 1965

**Cost to AEC:** \$11,000

**Contract Title:** THOMAS-FERMI MODEL FOR GRAPHITE

**Investigators:** George Handler

**Scope of Work:**

The objective of the project is to determine to what extent the statistical theory of quantum mechanical systems (Thomas-Fermi theory) may be reformulated so as to yield chemically useful information. Since accurate quantum mechanical calculations become impossible for all but the simplest systems, while statistical calculations are less difficult to do, this is a necessary study. We are examining alternate bases of representations and higher order approximations based on a product representation of an exponential function of the Hamiltonian operator. To date we have performed calculations on a number of atomic systems, with results in error by less than 8%, as compared to greater than 30% for ordinary Thomas-Fermi theory. We plan to extend these ideas and calculations to molecular and periodic systems. It is expected that the most powerful applications will be to problems of the solid state.

**Recent Publications:**

Sidney Golden and George S. Handler, "Continuous Representations in the Statistical Theory of Electronic Energies," J. of Chem. Physics, Vol. 39, No. 6 (1963), pp. 1543-1550.

Contractor: Utah, University of, Salt Lake City, Utah

Contract Number: AT(11-1)-1122

Present Contract Term: December 1, 1963 through November 30, 1964

Cost to AEC: \$14,061

Contract Title: RECRYSTALLIZATION AND SINTERING OF OXIDES

Investigators: Ivan B. Cutler

Scope of Work:

The objective of this project, to understand the effect of the impurities on the properties of ceramic oxides, has not changed over the past few years. Such processes as sintering grain growth, diffusion, electrical conductivity are decidedly altered by the impurity content. The results obtained thus far show that the diffusional processes concerned with aluminum oxide and magnesium oxide are more dramatically affected by impurity content than has been supposed at the beginning of the project. Electrical conductivity does not appear to be associated with diffusional processes, but it is likewise substantially altered by impurity contents.

The influence of small amounts of titanium dioxide on the rate of shrinkage of powder compacts of aluminum oxide was found to be truly remarkable. It has been possible to examine the limit of solid solution of titanium dioxide in aluminum oxide by sintering kinetics. A study of these kinetics has shown that small particles of alumina (less than one micron), doped with titanium dioxide, sintered by the bulk diffusion mechanism whereas large particles (greater than three microns), doped with titania, sintered by a grain boundary mechanism. This suggests that titanium ions in solid solution in the aluminum oxide lattice have a surface excess concentration which alters the kinetics of sintering.

The interdiffusion coefficient for  $Fe_xO$  diffusion into  $MgO$  is influenced by the chemical gradient as well as the diffusional gradient and was determined to be exponentially dependent upon the vacancy concentration. In order to study this phenomenon further, it was felt desirable to measure the interdiffusion coefficient in a system where it is possible to diffuse with a stoichiometric impurity as well as a non-stoichiometric impurity. Such a system is found with manganese oxide into magnesium oxide. By proper atmosphere control it is possible to alter the  $MnO$  from stoichiometric to non-stoichiometric. This project is well under way at the present time.

Solid solutions of FeO in MgO are excellent examples of crystalline materials with low electron mobility. Electrons travel through the lattice by hopping from one iron ion to another iron ion. This system is being studied further in order to delineate the influence of vacancies on the electron capture process. It is thought that electron holes associated with vacancies are rather immobile in comparison with holes that are free to hop through the crystal lattices.

**Contract:** University of Utah, Salt Lake City 12, Utah

**Contract Number:** AT(11-1)-1284

**Present Contract Term:** April 16, 1963 through August 14, 1964

**Cost to AEC:** \$21,917

**Contract Title:** A MAGNETIC RESONANCE STUDY OF DEFECTS IN SOLIDS

**Investigators:** William D. Ohlsen

**Scope of Work:**

The role of the hyperfine interaction in low-temperature spin-lattice relaxation will be experimentally studied by observing the effects of carbon isotopic substitution on the liquid-helium-temperature relaxation time of paramagnetic radiation-damage centers in Calcite. The hyperfine interaction information will also be used to study the structures of the Calcite radiation damage centers. Electron irradiation will be used for defect production.

A study of second-order-quadrupole NMR-line shifts in alkali-halide crystals will be continued. With KBr discrete Br lines quadrupole shifted by Na impurities have been seen and measured. The interpretation of these results is so far incomplete since the patterns obtained do not agree with those which should result from single Br sites such as (100) and (111) with respect to the Na. Experimental techniques limit the observable shifts to the range 15 kc to 80 kc. No lines have been found in this range for the system NaBr doped with K. Studies involving rotations about other than the (100) are planned as well as experiments involving spin mixing methods of detection.

A low-temperature electron-spin-resonance study of the donor Li in  $\text{TiO}_2$  will be conducted.

NOTICE OF RESEARCH PROJECT  
SCIENCE INFORMATION EXCHANGE  
SMITHSONIAN INSTITUTION

PROJECT NO. (Do not use this space)

KEY FOR PUBLICATION OR PUBLICATION REFERENCE
--

Division of Research

United States Atomic Energy Commission

SUPPORTING AGENCY:

TITLE OF PROJECT:

**"Interstitial Diffusion in Non-Metallic Crystals"**

Give names, departments, and official titles of PRINCIPAL INVESTIGATORS and ALL OTHER PROFESSIONAL PERSONNEL engaged on the project.

**Dr. Owen W. Johnson, Assistant Research Professor of Physics, Physics Department**

#15,041

NAME AND ADDRESS OF INSTITUTION:

**University of Utah, Salt Lake City, Utah 84112**

SUMMARY OF PROPOSED WORK -- (Approximately 200 words. Omit confidential data.) In the Science Information Exchange summaries of work in progress are exchanged with government and private agencies supporting research, and are forwarded to investigators who request such information. Your summary is to be used for these purposes. Please make your summary substantive in nature, rather than generally descriptive.

The proposed program of investigation is aimed at an eventual understanding of interstitial diffusion in non-metallic crystals. The study will begin by utilizing several unique characteristics of interstitial Li in rutile (TiO<sub>2</sub>) to permit measurement of the effect of hydrostatic pressure to 15 kbars on diffusion rates. It is also planned to measure Li isotope segregation, and to study diffusion of other interstitial species in this crystal. In support of the primary goal of the investigation and also to further the usefulness of this crystal as a "model" ceramic for a broad class of studies, an attempt will be made to develop techniques for growth of crystals of higher purity and perfection; studies of the electronic energy levels associated with various impurities are also planned.

Period for this RRP			
	to		
MO	YF	MO	YF
Sub-group			

SIGNATURE OF PRINCIPAL INVESTIGATOR

Identify the Professional School (medical, dental, public health, graduate, or other) with which this project should be identified.

SCHOOL

**Contract:** Vanderbilt University, School of Engineering,  
Nashville 5, Tennessee

**Contract Number:** AT(40-1)-3091

**Present Contract Term:** March 1, 1964 through February 28, 1965

**Cost to AEC:** \$16,172

**Contract Title:** DEFORMATION STUDIES OF SUPERLATTICE STRUCTURES

**Investigators:** J. J. Wert

**Scope of Work:**

The work hardening characteristics of superlattice alloys are known to differ greatly from those of systems which exhibit no long range order. In general it is believed that deformation will create new domain boundaries and destroy order through movement of dislocations on intersecting planes. Thus the effect of deformation is to decrease the domain size present in an alloy. Cohen and Bever of MIT have found that the Knoop hardness and yield strength of an initially ordered specimen increased more rapidly than that of initially disordered specimen as a function of plastic deformation. Presumably, the change in antiphase domain size due to plastic deformation enhances the materials resistance to plastic deformation. This investigation is designed to study the effects of deformation on  $\text{Cu}_3\text{Pt}$  in the ordered and disordered states in terms of the strain distribution<sup>3</sup> in different crystallographic directions, the antiphase domain size, and the particle size present as function of plastic deformation, and hence, the degree of order present. Whereas the  $\text{Cu}_3\text{Pt}$  alloy enables the study of the combined effects mentioned above, the independent effect of antiphase domain size will be investigated in the ordered b.c.c. superlattice of  $\text{Fe}_3\text{Al}$ . X-ray diffraction data will be analyzed via the method described by Averbach and Warren and will be correlated with mechanical properties wherever possible. It is anticipated that this investigation will yield fundamental knowledge concerning the deformation of superlattice structures.

Contractor: Vermont, University of, Burlington, Vermont

Contract Number: AT(30-1)-3000

Present Contract Term: October 1, 1963 through September 30, 1964

Cost to AEC: \$27,296

Contract Title: ABSORPTION OF HYDROGEN AND DEUTERIUM BY PALLADIUM-RICH ALLOYS

Investigators: Ted B. Flanagan

Scope of Work:

An investigation of the absorption of deuterium by a series of platinum/palladium alloys is near completion. The enthalpies, free energies and entropies of absorption of deuterium in the two-phase region of the 2.79, 5.73 and 8.80% platinum/palladium alloys have been determined. In addition relationships between relative resistance and deuterium content have been established and compared to the corresponding results for hydrogen.

Platinum/palladium alloys form a series of face centered cubic solid solutions. Although an expansion of the lattice occurs, the alloys retain a face centered cubic lattice after absorption of hydrogen or deuterium. Lattice constants have been determined at various hydrogen and deuterium contents.

It is planned to investigate the absorption of hydrogen and deuterium by a series of gold/palladium alloys during the coming contract year. Preliminary results indicate that the hydrogen/gold/palladium system will be of considerable interest. The free energy and enthalpy of absorption of hydrogen in the two-phase region passes through a maximum at small gold contents, approximately 6%. Relationships between the hydrogen content of these alloys and their relative resistances will be established.

Recent Publications:

T. B. Flanagan, "On Large Differences in the Equilibrium Solubilities of Hydrogen and Deuterium in Platinum-Palladium Alloys," J. Phys. Chem. 67, (1963) p. 203

**Contract:** Virginia Polytechnic Institute, Blacksburg, Virginia

**Contract Number:** AT(40-1)-2564

**Present Contract Term:** May 1, 1964 through April 30, 1965

**Cost to AEC:** \$15,029

**Contract Title:** FACTORS INFLUENCING THE FORMATION OF THE  $Cr_3O$ -TYPE STRUCTURE IN ALLOY SYSTEMS

**Investigators:** Roy C. Wilcox

**Scope of Work:**

Investigation of the Cr-Rh-Si system and the Nb-Al-Sn system will be initiated. The Cr-Rh-Si system will be studied to test the ability of B-atoms to substitute when both binary systems contain the  $Cr_3O$ -type structure. The Nb-Al-Sn systems will test the ability of a Group III<sup>3</sup> element to substitute for a Group IV element. The study of these systems will consist of a minimum of six alloys each with the compositions varying across the ternary systems at the 75 atom per cent line for the A-elements.

A study of the compatibility between the observed microstructure and X-ray diffraction will be conducted. Some alloys which are shown to be single phase as a result of X-ray analysis appear to be multi-phase when viewed metallographically. This apparent discrepancy may be the result of the inability to remove the as-melted dendritic structure.

The study of room temperature electrical resistivities in the V-Si-Sn and the Nb-Al-Sn systems will be undertaken. This study should help to give some information concerning the electronic structure of the  $Cr_3O$ -type structures.

**Contract:** Virginia Polytechnic Institute, Blacksburg, Virginia

**Contract Number:** AT(40-1)-2689

**Present Contract Term:** March 1, 1964 through February 28, 1965

**Cost to AEC:** \$34,051

**Contract Title:** THE PHYSICAL PROPERTIES OF CERIUM AS DETERMINED BY  
TEMPERATURE AND CRYSTAL STRUCTURE

**Investigators:** T. E. Leinhardt

**Scope of Work:**

Temperature and crystal structure dependencies of the electrical resistance and thermoelectric power of cerium are being examined to obtain information concerning imperfection and lattice scattering processes. Reflectivity measurements in the ultra-violet, visible and infra-red regions of the electromagnetic spectrum will be made to assist in the determination of the relative spacings of the various electronic levels lying close to the conduction bands. An analysis of absorptions in the infra-red region will aid in a study of the Stark splitting of the 4f level.

The theoretical part of our program is considering the application of the s-f exchange model to cerium. The model is being extended to include the effects of spin-orbit and crystal-field splitting of the 4f states.

Contractor: Virginia, University of, Charlottesville, Virginia

Contract Number: AT(40-1)-2488

Present Contract Term: February 1, 1964 through January 31, 1965

Cost to AEC: \$58,000

Contract Title: THE PROPERTIES OF CRYSTALLINE SOLIDS

Investigators: N. Cabrera

Scope of Work:

The program of research remains essentially the same as in preceding years, although some minor changes will be made in view of the fact that Dr. Mitchell is no longer one of our principal investigators.

We will continue work on the dislocation phenomena observed on thin ribbons of cadmium in the electron microscope. Furthermore, the studies on the deformation of copper alloys in the neighborhood of the yield point will be completed during the next years.

It is planned to continue and emphasize the work on surface problems both theoretically and experimentally. The equilibrium structure of crystal surfaces will be studied experimentally and the morphology of growing surfaces will be considered exclusively from theoretical point of view.

The epitaxial overgrowth and the properties of thin films will be studied and an effort will be made to relate the structural imperfection of the films to their electrical and other properties.

Finally, and paramount, we will study the dynamics of lattices at very low temperatures. This will include: Theoretical studies of the dynamics of imperfections in lattices; experimental studies on the electrical resistivity of metals under well controlled plastic deformation and subsequent annealing at higher temperatures; experimental studies on the resistivity under electron bombardment using a 1 MeV Van de Graaff, etc.

Recent Publications:

C. M. Drum and J. W. Mitchell, "Axial Dislocations in Thin Ribbons of Aluminum Nitride," Bull. Am. Phys. Soc. 8, FA, (1963) p. 204.

J. C. Crump and J. W. Mitchell, "Electron Microscope Studies of Fracture in Thin Ribbons of Cadmium," Bull. Am. Phys. Soc. 8, FA7, (1963) p. 204.

N. Cabrera and W. E. Atkinson, "Theory of the Motion of Imperfections in Lattices," Bull. Am. Phys. Soc. 8, FA9, (1963) p. 204.

J. W. Mitchell and E. E. Laufer, "New Observations of the Thermal Faceting of the Surfaces of Copper Crystals," Bull. Am. Phys. Soc. 8, OA2, (1963) p. 227.

E. Grunbaum and J. W. Mitchell, "Observations of Epitaxial Overgrowth of NiBr<sub>2</sub> on CrBr<sub>3</sub>," Bull. Am. Phys. Soc. 8, OA3, (1963) p. 227.

J. C. Crump and J. W. Mitchell, "Hexagonal Networks of Linear Imperfections in Single Crystals of Cadmium," Journ. Phys. Soc. Japan 18, (1963) p. 68.

J. C. Crump and J. W. Mitchell, "Hexagonal Networks of Linear Imperfections in Cadmium," Phil. Mag., London, 8, (1963) p. 59.

**Contract:** Virginia, University of, Charlottesville, Virginia

**Contract Number:** AT(40-1)-3012

**Present Contract Term:** June 1, 1964 through May 31, 1965

**Cost to AEC:** \$16,700

**Contract Title:** AN INVESTIGATION OF VACUUM-DEPOSITED SINGLE-CRYSTAL SEMICONDUCTOR FILMS

**Investigators:** Avery Catlin

**Scope of Work:**

The research proposed is a program of investigation into the causes of structural defects, mainly twins, observed in epitaxial germanium films, and the effects of these defects on the electrical properties of the films. Since these films are believed to be formed by individual crystalline nuclei growing together to finally produce a continuous film, experiments will be carried out to determine if the theory of nuclei misorientation offers an explanation for the formation of growth twins.

Once the source of these structural defects has been determined, such experimental techniques as vacuum cleaving of substrate crystals, slower deposition rates, and higher substrate temperatures will be investigated, in an effort to reduce the density of twins in vacuum-deposited germanium films. The effect of these defects on the electrical properties of the films will also be studied.

**Contract:** University of Virginia, Charlottesville, Virginia

**Contract Number:** AT(40-1)-3105

**Present Contract Term:** May 15, 1964 through May 14, 1965

**Cost to AEC:** \$30,158

**Contract Title:** ELECTRONIC PROPERTIES OF METALS AND ALLOYS

**Investigators:** Robert V. Coleman

**Scope of Work:**

Experimental research on the electric and magnetic properties of metals and alloys will continue under this program. Magnetoresistance and Hall effect measurements at liquid helium temperature have been carried out on copper, silver, zinc and cadmium under this program. These experiments are continuing and will be extended to include measurements in magnetic fields up to 50,000 gauss. Magnetoresistance and Hall effect measurements in dilute alloys of these metals are also underway. Field dependence and temperature dependence of resistance, magnetoresistance and Hall effect in both pure metals and alloys are being measured and analysis of the results in terms of scattering mechanisms and orbit topology is being carried out. Preliminary results of magnetoresistance and Hall effect in single crystal gold and silver films are also being obtained.

**Contract:** University of Virginia, Charlottesville, Virginia

**Contract Number:** AT(40-1)-3108

**Present Contract Term:** June 15, 1963 through September 14, 1964

**Cost to AEC:** \$6,900 (Supplemental for equipment)

**Contract Title:** INVESTIGATIONS ON THE BEHAVIOR OF POINT DEFECTS  
AND DISLOCATIONS

**Investigators:** Doris Kuhlmann-Wilsdorf

**Scope of Work:**

Four different topics of great scientific interest are to be studied:

- (i) By means of sensitive density measurements, determine the volume of relaxation of vacancies in metals. Further investigate the types and concentrations of point defects introduced into crystals through straining and irradiation treatments.
- (ii) Prepare and examine electrolytically deposited single crystal foils of gold and/or silver and investigate the mechanism by which crystal defects are formed in foils growing on substrates.
- (iii) Using a special furnace, grow aluminum crystals at an ambient temperature close to the melting point. Such crystals exhibit peculiar properties, presumably due to the lack of supersaturated vacancies. The phenomena associated with this are to be studied.
- (iv) Employing electro-deposition introduce thin distinguishable layers into single crystals and use these to trace the extent of slip bands in three dimensions.

The above projects are expected to throw new light on some controversial subjects such as (i) to which extent may slip line studies be employed in the development of theories on the workhardening of bulk specimens. (ii) What is the migration energy of interstitials in fcc metals, (iii) the origin of grown-in crystal defects.

Contractor: Virginia, University of, Charlottesville, Virginia

Contract Number: AT(40-1)-3109

Present Contract Term: May 1, 1964 through April 30, 1965

Cost to AEC: \$12,707

Contract Title: THE EARLY PHASES OF REACTIONS OF GASES ON METAL SURFACES

Investigators: Kenneth R. Lawless

Scope of Work:

The initial stages for the reaction of oxygen and oxygen plus hydrogen with copper are being studied by means of low-voltage electron diffraction. The first phase of this study involves the determination of the most suitable procedure for obtaining a single crystal surface which is as smooth, imperfection free and as clean as possible.

The second phase of this study concerns the determination of the structure of the adsorbed oxygen on the crystal surface. Also involved in this study is the mechanism of the solution of oxygen in the metal, and the relation of this solution to the formation of oxide nuclei. Rearrangement of surface metal atoms during the chemical reaction will be investigated.

Finally, the relationship between the orientation of adsorbed oxygen and of the final epitaxial oxide will be determined.

**Contract:** Wake Forest College, Winston-Salem, North Carolina

**Contract Number:** AT(40-1)-2413

**Present Contract Term:** May 15, 1964 through May 14, 1965

**Cost to AEC:** \$13,659

**Contract Title:** A STUDY OF ATOMIC MOVEMENTS IN SOLIDS EMPLOYING ANELASTIC AND RESISTIVITY MEASUREMENTS

**Investigators:** Thomas J. Turner  
George P. Williams, Jr.

**Scope of Work:**

Zener relaxation studies will continue in the AgAu, AgCd, AgIn, AgSb, and AgSn systems, yielding activation energies and jump rates for the processes as a function of the alloy concentration and crystal orientation. The quenching and resistivity measurements in the AgAu alloys to determine vacancy formation and migration energies are continuing complementary to the internal friction studies to provide even more information about this solid solution system. The ionic crystal work still has as its major objective the measurement of dislocation velocities and damping in lithium fluoride as a function of temperature, as well as to determine if the Granato-Lucke theory may legitimately be applied to ionic crystals. Finally, an answer to the question of the nature of stage III recovery following irradiation or cold work in metals is being sought. This should enable one to determine the interstitial configuration, which in turn should enable one to answer a more fundamental question, that of the nature of the potential function in fcc and bcc systems. The techniques of internal friction and resistivity will be used to study this problem specifically in platinum, nickel, tantalum, and chromium.

**Contract:** University of Washington, Seattle, Washington

**Contract Number:** AT(45-1)-1375

**Present Contract Term:** March 1, 1964 through February 28, 1965

**Cost to AEC:** \$17,712

**Contract Title:** PHASE TRANSFORMATIONS IN A EUTECTOID BINARY ALLOY SYSTEM

**Investigators:** Douglas H. Polonis

**Scope of Work:**

Work will be continued during the coming year on the study of metastable alloy phases. These studies are being conducted on high purity binary alloys prepared by the levitation melting technique. In one part of the program efforts are underway to resolve the overlapping reaction stages which complicate a quantitative analysis of the isothermal decomposition of martensite phases. Discontinuities which are being detected in some of the reaction curves derived from resistometric measurements must be identified with structural processes in order to resolve the effect of solute composition on the kinetics and mechanisms of the transformation. The effect of temperature on the rate of change of electrical resistivity at various stages of transformation is being explored as a method of determining the activation energies of the various reaction stages. An anomalous electrical resistance effect has been detected during cycling between  $-193^{\circ}\text{C}$  and  $100^{\circ}\text{C}$  in both the titanium metal and alloys used in this work; further studies to identify the mechanisms underlying this phenomenon are being included in the work for the coming year.

In the second phase of the program, work is in progress on the decomposition of high temperature phases with emphasis on the transition phase of the "omega" type. The omega phase will be studied to determine the mechanisms and kinetics of the transformation under conditions involved in quenching, aging, and applied stress. The experimental work will incorporate dilatometry, X-ray analysis, and electron microscopy techniques. In particular, electron microscopy thin film techniques are being explored as a means of investigating the role of crystal imperfections in the nucleation of transition phases in metastable alloys.

**Contract:** Wayne State University, Detroit, Michigan

**Contract Number:** AT(11-1)-1054

**Present Contract Term:** June 15, 1964 through August 14, 1965

**Cost to AEC:** \$35,800

**Contract Title:** ELECTRON PARAMAGNETIC RESONANCE STUDIES OF RADIATION EFFECTS IN SOLIDS AND CHEMICAL COMPOUNDS

**Investigators:** Yeong-Wook Kim

**Scope of Work:**

The purpose of the present work is to study the nature of radiation damage to several solids and chemical compounds.

The work on (i) alkali halides including LiF, (ii) lithium sulfate, (iii) organic compounds including diphenyl picryl hydrazine, and (iv) anti-ferromagnetic chromium sesqui-oxide and Ruby compounds will be further developed.

The investigations of these samples will be conducted by using the methods of electron paramagnetic resonance absorption, electron-nucleus double resonance absorption, and optical absorption. The temperature of the samples is expected to be controlled between 600 K and 1.5 K.

Neutrons, gamma-rays, and X-rays will be employed for the radiation treatments.

It is also planned to vary, as far as possible, the temperature of irradiation, the species of nuclear isotopes, oxygen pressure, and the type of solvents.

**Contractor:** West Virginia University, Morgantown, West Virginia

**Contract Number:** AT(40-1)-2839

**Present Contract Term:** September 1, 1963 through August 31, 1964

**Cost to AEC:** \$20,255

**Contract Title:** VOLUME MAGNETOSTRICTION OF FERROMAGNETIC MATERIALS

**Investigators:** Arthur S. Pavlovic

**Scope of Work:**

The magnetostriction of iron, cobalt and other ferromagnetic alloys are being investigated as a function of the magnetic field strength, over as wide a temperature range as possible. Particular attention is being given to the region about the curie temperature where the magnetization is changing rapidly. In addition, similar studies of single crystal and polycrystalline gadolinium and polycrystalline dysprosium metal are being carried out in the same manner. To supplement these studies with further information the magneto-caloric effect is being measured in the vicinity of the curie temperature for the above metals.

**Contract:** Western Reserve University, Cleveland, Ohio

**Contract Number:** AT(11-1)-1108

**Present Contract Term:** November 15, 1963 through November 14, 1964

**Cost to AEC:** \$31,000

**Contract Title:** ELECTRONIC SPECIFIC HEAT OF ALLOYS

**Investigators:** Ben A. Green, Jr.

**Scope of Work:**

The low-temperature specific heat of silver-based solid solutions are being measured in the range from 2 to 4°K. The main purpose of the experiments is to achieve high enough accuracy to measure reliably the slope of the curve of electronic specific heat coefficient ( $\gamma$ ) versus electron-per-atom ratio ( $e/a$ ). This goal has been achieved in the case of silver-tin alloys from 0 to 8 atomic percent tin. The silver-indium and silver-gold systems are now being investigated. The most interesting conclusion to be drawn from the silver-tin results is that silver acts like a free-electron gas both with respect to its  $\gamma$  value (0.646 millijoules per mole per deg<sup>2</sup> compared to the free-electron value of 0.644) and the slope mentioned above (0.15 in the same units compared to the free-electron value of 0.215). The slope disagrees with the prediction of Ziman (-0.595). Its dependence on valence of solute may be seen by comparison with the silver-cadmium data of Montgomery and Pells. The slope is proportional to the valence difference between solvent and solute, in disagreement with the recent theory of Jones which predicts a proportionality to the square of this valence difference. Liquid alloy resistivities are also being investigated to explore reported anomalies in the concentration dependence of the excess resistivity.

**Contract:** Western Reserve University, Cleveland, Ohio

**Contract Number:** AT(11-1)-1146

**Present Contract Term:** March 1, 1964 through February 28, 1965

**Cost to AEC:** \$42,000

**Contract Title:** RECOIL-FREE SCATTERING OF GAMMA RAYS

**Investigators:** John K. Major

**Scope of Work:**

The recoil-free scattering of gamma rays from solids and liquids is being studied by using the Mössbauer effect as an energy analyzer. Phase transitions between the solid and liquid states will be studied, and the relative amounts of recoil-free scattering from linear and cross-linked polymers will be measured. From determinations of the Debye-Waller factor, an effective Debye temperature will be deduced as a function of scatterer temperature, yielding information on the phonon excitation spectrum not otherwise readily available. Information on the self-diffusion coefficient will be obtained from determinations of the line width of the recoil-free scattering. The importance of local order and, in particular, molecular linkage in making recoil-free scattering possible will be explored in these experiments. In addition, recoil-free resonant absorption and scattering in rare earths and their compounds will be studied.

The velocity modulation system for use in displaying velocity spectra on a multichannel analyzer is being completed, and preliminary tests have been made on various source-absorber combinations to maximize the Mössbauer effect and to minimize the line width, isomeric shift, and photoabsorption in the absorber. Measurements of the angular dependence of resonant scattering from stainless steel with equal incident and emergent angles show agreement with earlier results, but a discrepancy with the calculated values which will be further explored.

**Contract:** Western Reserve University, Cleveland, Ohio

**Contract Number:** AT(11-1)-1297

**Present Contract Term:** June 15, 1964 through June 14, 1965

**Cost to AEC:** \$32,500

**Contract Title:** POSITRON ANNIHILATION IN LIQUIDS AND SOLIDS

**Investigators:** John D. McGervey

**Scope of Work:**

A. Measurement of mean lives of positrons in metals

The objective of this project is to measure mean lives of positrons in many metals for which accurate measurements of this sort have not been made. These results will be correlated with the valence electron densities in the various metals and with results of angular correlation measurements on the annihilation gamma rays. Although no theoretical model exists which gives really good agreement with present data, a successful theory should help in the understanding of the effects of impurities in metals.

B. Measurement of the correlation between the positron lifetime and the angle between the annihilation gamma rays

In amorphous materials the distribution of the angles between the positron annihilation gamma rays is strongly peaked at  $180^\circ$ . The object of this project is to establish the connection between this "narrow component" and the long-lived component in the positron lifetime distribution. It is believed that the narrow component in the angular distribution comes from the annihilation of thermalized singlet positronium, while the long-lived component comes from annihilation of positrons which originally formed triplet positronium. It has often been suggested in the past six or seven years that this connection should be investigated directly by a simultaneous measurement of lifetime and angle but only recently have fast electronic techniques become available which make this possible.

C. Measurement of electron momentum distributions in metals by positron annihilation

The objective of this project is to measure directly the momentum distributions of electrons in various materials, by measuring the angular correlation of gamma rays from positron annihilations in these materials.

This angular correlation is measured by counting coincidences between pulses in two detectors placed on opposite sides of the sample in which the annihilations occur. A long narrow slit in front of each detector defines the gamma ray directions. These directions are changed and the number of coincidence counts are recorded automatically at preset time intervals. At present each slit is 1 mm wide and at a distance of 2 m from the sample, so that the angular resolution is  $\pm 1/2$  milliradian. The half-width of the angular distributions varies from  $\bar{5}$  to 10 milliradians.

**Contract:** Westinghouse Electric Corporation, Pittsburgh 35,  
Pennsylvania

**Contract Number:** AT(30-1)-3203

**Present Contract Term:** June 1, 1964 through May 31, 1965

**Cost to AEC:** \$46,274

**Contract Title:** REACTIONS OF HYDROGEN WITH ALLOYS OF ZIRCONIUM

**Investigators:** Earl A. Gulbransen

**Scope of Work:**

The objective of this program is to study the reaction of zirconium alloys of the first long period of the periodic table with oxygen, water vapor plus oxygen, and water vapor plus traces of oxygen. A flow system will be used and the reaction gases monitored. Temperatures between 300°C and 600°C will be used. The extent of oxidation and the resulting hydrogen picked up will be measured for several time intervals. The crystal structure and microstructure of the oxide layers will be determined. The effect of oxidation on the metal structure also will be determined.

Equilibrium and kinetic studies will be made of the hydrogen reaction on oxide free surfaces of the alloys. Direct hydrogen penetration of oxidized alloys also will be studied.

Two compositions in each of the following alloy systems will be studied Zr-V, Zr-Cr, Zr-Fe, Zr-Co, Zr-Ni, Zr-Cu and Zr-Mo. The two compositions will be the eutectoid compositions and the first intermetallic (ZrV<sub>2</sub>, ZrCr<sub>2</sub>, ZrFe<sub>2</sub>, ZrCo<sub>2</sub>, Zr<sub>2</sub>Ni, Zr<sub>2</sub>Cu, and ZrMo<sub>2</sub>).

It is hoped to relate the hydrogen pickup to the equilibrium hydrogen-alloy phase diagram and to the nature, structure, and composition of the oxide film formed during oxidation in water vapor atmospheres.

**Contract:** Wisconsin, University of, Madison, Wisconsin

**Contract Number:** AT(11-1)-987

**Present Contract Term:** February 1, 1964 through January 31, 1965

**Cost to AEC:** \$13,808

**Contract Title:** DEFECT PHASES IN ALLOYS

**Investigators:** R. A. Dodd

**Scope of Work:**

Dislocation configurations in alloys corresponding to the defective and non-defective regions of the B NiAl (CsCl structure) are being examined using thin-film transmission electron microscopy. The results will be correlated with published information on strength and deformation characteristics of this phase.

Alloys in the gamma phase (21/13 electron compounds) regions of the Ni-Zn and Au-Zn systems have been prepared, substantially by vapor diffusion methods. The electron concentration at which the phases become defective is being determined by an analysis of discrepancies between theoretical and actual densities.

The initial dislocation densities and distributions in pure metal and solid solution single crystals will be determined as a function of method of crystal preparation. The preparation methods will include, 1) solidification from the melt, 2) recrystallization, and 3) vapor diffusion of one component into a single crystal of the second component. The results will be related to theories of solid solution hardening.

Recent Publications:

W. J. Helfrich and R. A. Dodd, "A Reconsideration of the Evidence for the Existence of Anomalously High Concentrations of Vacancies in Alloy Phases Acta. Met. Vol. II, No. 8, (1963) pp. 982-986.

Paul W. McDaniel, Director  
Division of Research

November 9, 1964

Mark C. Wittels, Metallurgy and Materials  
Programs, Division of Research

**NEW CONTRACT WITH THE UNIVERSITY OF WISCONSIN (MAYNARD/VOGELSANG)**

A proposal entitled "Radiation Interactions in Solids; Surface and High Pressure Effects" has been received and reviewed. Initially the proposal was for research in three areas: (a). radiation damage at high pressure, (b). radiation damage to solid surfaces, and (c). neutron diffraction at high pressure.

Radiation damage studies at high pressure are nearly untouched regions of research and some important questions need to be answered concerning the physical effects of these combined, simultaneous processes. Since pressures of 100 kilobars can compress crystal structures up to 20% it is curious to contemplate how this might affect the potential barrier or displacement threshold in the radiation damage process. Equally interesting is the possibility of driving phase transformations by the combined processes, and an initial study is proposed for graphite diamond utilizing an anvil pressure cell capable of pressures up to 100 kilobars. Early efforts will also be directed towards phase transitions in zirconium dioxide, and possibly, later, some other solids, in which fast neutron-induced transitions have already been produced by others. The pressure cell, and X-ray and electron microscope equipment is already available for these studies but modest funds are requested for a microtome and micromanipulator for handling small samples.

In the surface study portion of the program the ultra-high vacuum system and mass spectrometer is in a readiness condition for the first experiments. These studies will be with irradiated and unirradiated crystals of germanium and silicon that will be cleaved under high vacuum to avoid surface contamination. Following electrical measurements on these specimens gases will be entered into the system and the mass spectrometer will be utilized to measure gas compositions in several exchanges and decompositions. The objective of this research is to obtain a better understanding of the role of defects in catalytic activity and to correlate results with electrical and chemical properties of surfaces. Again, as in the first area of this proposal little research has been done, and a relatively untouched field is open.

The third study in the proposal involves neutron diffraction at high pressures, a field which is just beginning to receive increasing

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attention. It was noted at the onset that the investigators had no experience in this area and this view was confirmed by outside review. As a result I requested that this section of the proposal be dropped until one or both of the investigators gained experience, possibly during the summer, at one of the national laboratories. Negotiations for this are now being made at ANL and EML by Professor Vogelsang.

The proposal received favorable reviews in the first two studies, and it was suggested that considerable imagination and resourcefulness was displayed by the co-investigators. Reviewers included Drickamer (Ill.), Wollan (ORNL), Shull (MIT) and Lawson (Calif.). It is anticipated that the AEC will soon license the 1 Mw operation of the Wisconsin reactor and this will considerably speed the research. The investigators previous reactor experience should certainly assist their efforts in this program. They have no other federally supported research.

The studies are definitely in AEC interests and support is recommended as indicated in the revised budget.

New AEC funds	\$55,884
Wisconsin funds	4,000
<b>TOTAL</b>	<b>\$59,884</b>

Title to the equipment should be vested in the university, since the nature of the equipment and the institution's research program make it reasonable to expect that the equipment will be devoted to research or training programs of interest to the AEC after the termination of AEC support.

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**Contract:** Yale University, New Haven, Connecticut

**Contract Number:** AT(30-1)-2560

**Present Contract Term:** April 1, 1964 through March 31, 1965

**Cost to AEC:** \$19,936.00

**Contract Title:** X-RAY STUDY OF THE STRUCTURE OF LIQUID METALS AND ALLOYS

**Investigators:** Christian N. J. Wagner

**Scope of Work:**

1. Structure of Molten Binary Alloys

Molten silver-tin alloys have been studied with a focusing  $\theta$ - $\theta$  diffractometer. The interference function  $I(K) = I_{eu}/f^2$  have been measured in the range of  $K = 4\pi \sin\theta/\lambda = 1.4\text{\AA}^{-1}$  to  $K = 15\text{\AA}^{-1}$  at about  $100^\circ\text{C}$  above the liquidus temperature for eight different compositions. The position of the first maximum in the radial distribution function, obtained by Fourier transforms of  $I(K)$ , is a measure of the interatomic distance  $r_1$  in the molten alloys. The plot of  $r_1$  versus alloy composition shows a negative deviation from a linear law.

The molten alloys of Sn-In and Hg-Tl are being investigated. In addition, it seems of interest to study the system Te-In which has been investigated in the metastable amorphous state obtained by rapid quenching from the liquid.

2. Structure of Molten Metals

The interference functions and radial distribution functions of Cu, Ag, Sn, and Hg were obtained from x-ray diffraction data.

The interatomic distances  $r_1$  in these metals correspond very closely to their Goldschmidt diameters. The metals Zn, Cd, and Hg are being investigated in the molten state as a function of temperature.

Contractor: Yale University, New Haven, Connecticut

Contract Number: AT(30-1)-2723

Present Contract Term: January 1, 1964 through December 31, 1965

Cost to AEC: \$23,965

Contract Title: THE STRUCTURE AND ASSOCIATED PROPERTIES OF IONIC SOLID SOLUTIONS

Investigators: W. D. Robertson

Scope of Work:

The factors defining the stability of solid solutions in ionic systems are being studied. In particular single crystal elastic moduli. Thermal expansion and x-ray intensity data are being obtained for the two systems KF-RbF and KI-RbI, which represent systems of homogeneous solid solutions exhibiting the maximum differences in cohesive parameters of the pure components.

Simultaneously, a study of the original literature (over 500 pagers) pertaining to binary phase diagrams of ionic systems is being made with the objective of compiling a set of critically evaluated phase diagrams to use in subsequent research.

**Contract:** Yale University, New Haven, Connecticut

**Contract Number:** AT(30-1)-3227

**Present Contract Term:** June 1, 1964 through May 31, 1965

**Cost to AEC:** \$98,933.00

**Contract Title:** THE STUDY OF IDEAL MAGNETIC CRYSTALS

**Investigators:** Werner P. Wolf

**Scope of Work:**

The objective of this work is detailed understanding of the magnetic and thermal properties of selected materials, carefully chosen to be "ideal" from the point of view of being describable in simple and unambiguous terms. The materials at present under investigation are mainly insulating rare earth compounds.

Facilities have been developed for the preparation of single crystals from aqueous solution (ethyl sulphates), high temperature flux, (garnets), and by the Bridgeman method (chlorides). A Czochralski crystal pulling unit is now being constructed.

Experimental investigations include precision susceptibility measurements at low temperatures, (inductance method), magnetization measurements (vibration magnetometer) and ESR at 9 and 25 KMc/s. An apparatus for making accurate magnetic and thermal measurements in the temperature range  $0.1^{\circ}\text{K}$  to  $1^{\circ}\text{K}$  is currently being planned.

The systems being studied include i)  $\text{Dy}_3\text{Al}_5\text{O}_{12}$ , an extremely anisotropic antiferromagnet, whose properties are closely related to those of theoretical Ising models, ii)  $\text{GdCl}_3$  one of the few known ferromagnetic insulators, whose properties are dominated by the unusually large ratio of magnetic to exchange interaction, iii) Interacting pairs of magnetic ions in non-magnetic lattices, specifically rare earths in hexagonal trichlorides, iv) ESR spectra of single ions in crystals with temperature independent paramagnetism which show the recently discovered g-value exchange shift.

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